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				STN Express with Discover!								
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NEWS	5	NOV		PHAR reloaded with additional data								
NEWS	6	DEC		LISA now available on STN								
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NEWS	8	DEC	15	MEDLINE update schedule for December 2004								
NEWS	9	DEC	17	ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected								
NEWS	10	DEC	17	COMPUAB reloaded; updating to resume; current-awareness								
				alerts (SDIs) affected								
NEWS	11	DEC	17	SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected								
NEWS	12	DEC	17	CERAB reloaded; updating to resume; current-awareness								
				alerts (SDIs) affected								
NEWS	13	DEC	17	THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB								
NEWS	14	DEC	30	EPFULL: New patent full text database to be available on STN								
NEWS	15	DEC	30	CAPLUS - PATENT COVERAGE EXPANDED								
NEWS	16	JAN	03	No connect-hour charges in EPFULL during January and								
				February 2005								
NEWS	17	FEB	25	CA/CAPLUS - Russian Agency for Patents and Trademarks								
				(ROSPATENT) added to list of core patent offices covered								
NEWS	18	FEB	10	STN Patent Forums to be held in March 2005								
NEWS	19	FEB	16	STN User Update to be held in conjunction with the 229th ACS								
				National Meeting on March 13, 2005								
NEWS	20	FEB	28	PATDPAFULL - New display fields provide for legal status								
				data from INPADOC								
NEWS		FEB		BABS - Current-awareness alerts (SDIs) available								
NEWS		FEB		MEDLINE/LMEDLINE reloaded								
NEWS		MAR		GBFULL: New full-text patent database on STN								
NEWS		MAR		REGISTRY/ZREGISTRY - Sequence annotations enhanced								
NEWS	25	MAR	03	MEDLINE file segment of TOXCENTER reloaded								
NEWS EXPRESS			NUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT									
<u>Μ</u> Δ		MA( ANI	ACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), ND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005									
				,								
-				N Operating Hours Plus Help Desk Availability								
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				come Banner and News Items								
				rect Dial and Telecommunication Network Access to STN								
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SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 14 MAR 2005 HIGHEST RN 845540-96-7 DICTIONARY FILE UPDATES: 14 MAR 2005 HIGHEST RN 845540-96-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10807612.str

#### L1 STRUCTURE UPLOADED

STR

=> d l1

L1 HAS NO ANSWERS

L1 .

G1 C,O,N

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 19:45:16 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2914 TO ITERATE

34.3% PROCESSED 1000 ITERATIONS

9 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

55043 TO 61517

PROJECTED ANSWERS:

217 TO 831

L2

9 SEA SSS SAM L1

=> search l1

ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:. ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full FULL SEARCH INITIATED 19:45:23 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 57686 TO ITERATE

100.0% PROCESSED 57686 ITERATIONS

611 ANSWERS

SEARCH TIME: 00.00.02

L3 611 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST

161.33 161.54

FILE 'CAPLUS' ENTERED AT 19:45:38 ON 15 MAR 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 15 Mar 2005 VOL 142 ISS 12 FILE LAST UPDATED: 14 Mar 2005 (20050314/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4 83 L3

### => dl4 1-83

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### => d 14 1-83 fbib ab hitstr

- L4 ANSWER 1 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 2004:1068183 CAPLUS
- DN 142:177109
- TI A solid phase linker strategy for the direct synthesis of EDANS-labeled peptide substrates
- AU Beythien, Joerg; White, Peter D.
- CS Novabiochem, Merck Biosciences AG, Laufelfingen, CH-4448, Switz.
- SO Tetrahedron Letters (2004), Volume Date 2005, 46(1), 101-104 CODEN: TELEAY; ISSN: 0040-4039
- PB Elsevier B.V.
- DT Journal
- LA English
- AB A novel linker strategy for the efficient synthesis of peptides C-terminally labeled with the EDANS [EDANS = 1-Naphthalenesulfonic acid, 5-[(2-aminoethyl)amino]-] fluorophore is described. Using this support, FRET peptide substrates bearing EDANS/Dabcyl [Dabcyl = benzoic acid, 4-[[4-(dimethylamino)phenyl]azo]-] fluorescent donor/acceptor groups can be readily prepared using standard Fmoc (Fmoc = 9-fluorenylmethyloxycarbonyl) solid phase methods.
- IT 832731-23-4P
  - RL: SPN (Synthetic preparation); PREP (Preparation) (solid phase synthesis of EDANS-labeled peptides)
- RN 832731-23-4 CAPLUS
- CN L-Leucinamide, 1-[4-[[4-(dimethylamino)phenyl]azo]benzoyl]-L-prolyl-Ltyrosyl-L-tyrosylglycyl-L-α-aspartyl-L-α-glutamyl-L-prolyl-N[2-[(5-sulfo-1-naphthalenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

PAGE 1-A

# RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:817911 CAPLUS

DN 141:327647

TI Fluorogenic peptides substrates for PHEX endopeptidase and their use for PHEX detection and quantitation and in screening for PHEX modulators

IN Boileau, Guy; Carmona, Adriana Karaoglanovic; Campos, Marcelo; Juliano, Maria Aparecida; Juliano, Luiz

PA Biomep Inc., Can.

SO PCT Int. Appl., 56 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN. CNT 1

	PATENT	KIND		DATE			APPLICATION NO.						DATE				
						-									-		
ΡI	WO 2004	WO 2004085465					2004	1007	WO 2004-CA453					20040325			
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
							DE,										

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GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
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US 2003-457296P

P 20030326

OS MARPAT 141:327647

Fluorogenic peptide substrates are provided for PHEX endopeptidase. fluorogenic PHEX substrates comprising a peptide unit, a fluorophore unit (e.g., 3-aminobenzoic acid [Abz]) capable of conferring fluorescence on said substrate attached to an amino acid residue at a first end of the peptide unit, and a quencher unit (2,4-dinitrophenyl [Dnp] or 2,4-dinitrophenyl-ethylenediamine [EDDnp]) capable of providing intramol. quenching of said fluorescence attached to an amino acid residue at a second end of the peptide unit. The peptide unit has at least 6 amino acids residues including a sequence P2-P1-P1'-P2' of 4 amino acid residues: the amino acid residue at position P2 is any amino acid residue; the amino acid residue at position P1 is any amino acid residue except an isoleucine, a valine, or a histidine residue; the amino acid residue at position P1' is an acidic amino acid residue selected from the group consisting of a glutamic acid residue and an aspartic acid residue, and being located at least 2 amino acid residues distal to both the fluorophore and the quencher units; and the amino acid residue at position P2' is any amino acid residue except a leucine, a proline or a glycine residue, with the proviso that said peptide unit does not have the sequence Ala-Trp-Leu-Asp-Ser-Gly-Val. Internally quenched fluorogenic peptides are identified kinetic anal. using positional scanning synthetic combinatorial peptide libraries and putative natural libraries based on the sequences of parathyroid hormone-related peptide (PTHrP), fibroblast growth factor-23 (FGF23), and matrix extracellular phosphoglycoprotein (MEPE); neprilysin-based peptides are not hydrolyzed by PHEX. At least 3 fluorogenic substrates are good soluble PHEX substrates for determination of

PHEX

AΒ

activity and concentration in serum: Abz-GFRDWK-Dnp, Abz-DHLSDTSTQ-EDDnp, and Abz-GFSDYK-Dnp. Methods of using the peptide sequence unit to identify PHEX modulators are also provided.

TT 767337-81-5 767337-87-1 767337-88-2 767337-89-3

RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);
ANST (Analytical study); BIOL (Biological study); USES (Uses)
(fluorogenic peptides substrates for PHEX endopeptidase and their use
for PHEX detection and quantitation and in screening for PHEX
modulators)

RN 767337-81-5 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)glycyl-L-phenylalanyl-L-seryl-L-αaspartyl-L-tyrosyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA
INDEX NAME)

$$NO_2$$
 $NO_2$ 
 $NO_2$ 

PAGE 1-B

$$\begin{array}{c|c}
 & H \\
 & N \\
 & H \\
 & Ph \\
\end{array}$$

RN 767337-87-1 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)-L-seryl-L-alanyl-L- $\alpha$ -glutamyl-L- $\alpha$ -aspartyl-L-asparaginyl-L-seryl-L-prolyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 767337-88-2 CAPLUS

CN L-Glutamamide, N2-(2-aminobenzoyl)-L-arginyl-L-seryl-L- $\alpha$ -glutamyl-L- $\alpha$ -aspartyl-L-alanylglycyl-L-phenylalanyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RN 767337-89-3 CAPLUS

CN L-Glutamamide, N2-(2-aminobenzoyl)-L-asparaginylglycyl-L-tyrosyl-L- $\alpha$ -aspartyl-L-valyl-L-tyrosyl-L-histidyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-B

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 3 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 2004:817666 CAPLUS
- DN 141:309638
- TI Inhibitors of cathepsin S for use in disease treatment
- IN Liu, Hong; Tully, David; Epple, Robert; Bursulaya, Badry; Williams, Jennifer; Chatterjee, Arnab; Harris, Jennifer Leslie; Li, Jun
- PA IRM LLC, Bermuda
- SO PCT Int. Appl., 146 pp.

CODEN: PIXXD2

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DT
     Patent
LΑ
     English
FAN.CNT 1
                           KIND
                                  DATE
                                               APPLICATION NO.
                                                                        DATE
     PATENT NO.
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     ______
                           ----
                                                                        20040324
                                               WO 2004-US9218
PΙ
     WO 2004084842
                            A2
                                  20041007
     WO 2004084842
                           A3
                                  20041125
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
         W:
              CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
              LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
              NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
              TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
              BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
              ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
              SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
                                               US 2003-457595P
                                                                        20030324
                                               US 2004-807612
                                                                        20040323
     US 2004198780
                            A1
                                  20041007
                                               US 2004-807612
                                                                        20040323
```

OS MARPAT 141:309638

AB The present invention provides WC(:0)NHCH2CH2NHAr [W = R1X(C:0)NHCHR2; R1 = (substituted)phenyl, pyridyl, or pyridinium N-oxide; X = furan, NHCH2, OCH2, phenylene, etc.; R2 = (substituted)phenyl, etc.; Ar = (substituted phenyl)] compds. and methods for the selective inhibition of cathepsin S. In a preferred aspect, cathepsin S is selectively inhibited in the presence of at least one other cathepsin isoenzyme (e.g., cathepsin K). The present invention also provides methods for treating a disease state in a subject by selectively inhibiting cathepsin S.

US 2003-457595P

ΙT 768363-56-0P 768363-57-1P 768363-58-2P 768363-59-3P 768363-60-6P 768363-61-7P 768363-62-8P 768363-63-9P 768363-64-0P 768363-65-1P 768363-66-2P 768363-67-3P 768363-68-4P 768363-69-5P 768363-70-8P 768363-71-9P 768363-72-0P 768363-73-1P 768363-74-2P 768363-75-3P 768363-76-4P 768363-77-5P 768363-78-6P 768363-79-7P 768363-80-0P 768363-81-1P 768363-82-2P 768363-83-3P 768363-84-4P 768363-85-5P 768363-86-6P 768363-87-7P 768363-88-8P 768363-89-9P 768363-90-2P 768363-91-3P 768363-92-4P 768363-93-5P 768363-94-6P 768363-95-7P 768363-96-8P 768363-97-9P 768363-98-0P 768363-99-1P 768364-00-7P 768364-01-8P 768364-02-9P 768364-03-0P 768364-04-1P 768364-05-2P 768364-06-3P 768364-07-4P 768364-08-5P 768364-09-6P 768364-10-9P 768364-11-0P 768364-12-1P 768364-13-2P 768364-14-3P 768364-15-4P 768364-16-5P 768364-17-6P 768364-18-7P 768364-19-8P 768364-20-1P 768364-21-2P 768364-22-3P 768364-23-4P 768364-24-5P 768364-25-6P 768364-27-8P 768364-28-9P 768364-29-0P 768364-30-3P 768364-31-4P 768364-32-5P 768364-33-6P 768364-34-7P 768364-35-8P 768364-36-9P 768364-37-0P 768364-38-1P 768364-39-2P 768364-40-5P 768364-42-7P 768364-43-8P 768364-45-0P

Appliants.

20030324

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768364-46-1P 768364-47-2P 768364-48-3P
768364-49-4P 768364-50-7P 768364-51-8P
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768364-55-2P 768364-56-3P 768364-57-4P
768364-58-5P 768364-59-6P 768364-60-9P
768364-61-0P 768364-62-1P 768364-63-2P
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768364-67-6P 768364-68-7P 768364-69-8P
768364-70-1P 768364-71-2P 768364-72-3P
768364-73-4P 768364-74-5P 768364-75-6P
768364-76-7P 768364-77-8P 768364-78-9P
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768365-18-0P 768365-19-1P 768365-20-4P
768365-21-5P 768365-22-6P 768365-23-7P
768365-24-8P 768365-25-9P 768365-26-0P
768365-27-1P 768365-28-2P 768365-29-3P
768365-30-6P 768365-31-7P 768365-32-8P
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768365-84-0P 768365-85-1P 768365-86-2P
768365-87-3P 768365-88-4P 768365-89-5P
768365-90-8P 768365-91-9P 768365-92-0P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (inhibitors of cathepsin S for use in disease treatment)
768363-56-0 CAPLUS
2-Furancarboxamide, N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]car
bonyl]-3-phenylpropyl]-5-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX
NAME)
```

Absolute stereochemistry.

RN

CN

RN 768363-57-1 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-[(2-chlorophenyl)methyl]-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-5-[3-(trifluoromethyl)phenyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$F_3C$$

$$N_1 S$$

$$N_2 S$$

$$N_1 S$$

$$N_1 S$$

$$N_2 S$$

$$N_3 S$$

$$N_1 S$$

$$N_1 S$$

$$N_2 S$$

$$N_3 S$$

$$N_1 S$$

$$N_1 S$$

$$N_2 S$$

$$N_3 S$$

$$N_3 S$$

$$N_4 S$$

$$N_1 S$$

$$N_1 S$$

$$N_2 S$$

$$N_3 S$$

$$N_4 S$$

$$N_1 S$$

$$N_1 S$$

$$N_2 S$$

$$N_3 S$$

$$N_4 S$$

$$N_1 S$$

$$N_1 S$$

$$N_2 S$$

$$N_3 S$$

$$N_4 S$$

$$N_5 S$$

RN 768363-58-2 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-[(3-chlorophenyl)methyl]-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-5-[3-(trifluoromethyl)phenyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-59-3 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-[(4-chlorophenyl)methyl]-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-5-[3-(trifluoromethyl)phenyl]-(9CI) (CA INDEX NAME)

RN 768363-60-6 CAPLUS

CN 2H-Pyran-4-propanamide, tetrahydro-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[[[5-[3-(trifluoromethyl)phenyl]-2-furanyl]carbonyl]amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-61-7 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-(cyclopentylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-5-[3-(trifluoromethyl)phenyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$F_3C$$

$$H$$

$$N$$

$$H$$

$$N$$

$$H$$

$$N$$

$$H$$

$$S$$

RN 768363-62-8 CAPLUS

CN Benzenepropanamide,  $4-(2,3-\text{dimethylphenoxy})-N-[2-[(4-\text{methoxyphenyl})\,\text{amino}]\,\text{ethyl}]-\alpha-[(3-\text{methylbenzoyl})\,\text{amino}]-, (\alpha S)-(9CI) (CA INDEX NAME)$ 

RN 768363-63-9 CAPLUS

CN Benzeneacetamide, 4-chloro-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} C1 \\ \hline \\ NH-CH_2-CH_2-NH-C-CH-NH-C \\ \hline \\ MeO \end{array}$$

RN 768363-64-0 CAPLUS

CN 2-Furancarboxamide, N-[2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxo-1-phenylethyl]-5-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 768363-65-1 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[[4-(difluoromethoxy)phenyl]amino]ethyl]amino]-2-oxoethyl]-5-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

$$F_3$$
C  $H$   $N$   $H$   $N$   $H$   $N$   $H$   $N$   $H$ 

RN 768363-66-2 CAPLUS

CN Benzoic acid, 4-[[2-[[(2S)-3-cyclohexyl-1-oxo-2-[[[5-[3-(trifluoromethyl)phenyl]-2-furanyl]carbonyl]amino]propyl]amino]ethyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-67-3 CAPLUS

CN Benzoic acid, 2-[[2-[[(2S)-3-cyclohexyl-1-oxo-2-[[[5-[3-(trifluoromethyl)phenyl]-2-furanyl]carbonyl]amino]propyl]amino]ethyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-68-4 CAPLUS

CN Benzeneacetamide, N-[(1S)-3-cyclohexyl-1-[[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]carbonyl]propyl]-α-methyl-, (αR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-69-5 CAPLUS

CN 4-Piperidinecarboxamide, 1-acetyl-N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-

[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-70-8 CAPLUS

CN Cyclohexanepropanamide,  $\alpha$ -[[[4-(4-acetyl-1-piperazinyl)phenoxy]acetyl]amino]-N-[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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RN 768363-71-9 CAPLUS

CN Benzenepropanamide,  $\alpha$ -[(2-chloro-3-methylbenzoyl)amino]-N-[2-[(4-methoxyphenyl)amino]ethyl]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 768363-72-0 CAPLUS

CN Benzeneacetamide, N-[1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-4-methoxy- (9CI) (CA INDEX NAME)

$$\begin{picture}(20,0) \put(0,0){\line(1,0){0.5ex}} \put(0,0){\line(1,0){0.5ex$$

RN 768363-73-1 CAPLUS

CN [1,1'-Biphenyl]-4-propanamide, 3',5'-dichloro-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-74-2 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-4-(methylsulfonyl)-(9CI) (CA INDEX NAME)

RN 768363-75-3 CAPLUS

CN Benzenepropanamide,  $\alpha$ -[[3,5-dimethyl-4-(phenylmethoxy)benzoyl]amino]-N-[2-[(4-methoxyphenyl)amino]ethyl]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-76-4 CAPLUS

CN Benzenepropanamide,  $\alpha$ -[(4-methoxy-3,5-dimethylbenzoyl)amino]-N-[2-[(4-methoxyphenyl)amino]ethyl]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-77-5 CAPLUS

CN 1H-Indole-2-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-methoxy- (9CI) (CA INDEX NAME)

RN 768363-78-6 CAPLUS

CN 2-Furancarboxamide, 5-(3-fluorophenyl)-N-[(1S)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxo-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-79-7 CAPLUS

CN Benzenepropanamide,  $\alpha$ -[(3-bromo-4-methylbenzoyl)amino]-N-[2-[(4-methoxyphenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 768363-80-0 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 768363-81-1 CAPLUS

CN 2-Thiophenecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-82-2 CAPLUS

CN 3-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-83-3 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-4-(5-methyl-1,2,4-oxadiazol-3-yl)- (9CI) (CA INDEX NAME)

RN 768363-84-4 CAPLUS

CN 2-Thiophenecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-(4-fluorophenyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-85-5 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(2,4,5-trimethylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-86-6 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-(3-fluorophenyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-87-7 CAPLUS

CN 2-Morpholinecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-88-8 CAPLUS

CN Benzenepropanamide,  $4-[4-(dimethylamino)phenoxy]-N-[2-[(4-methoxyphenyl)amino]ethyl]-<math>\alpha-[(3-methylbenzoyl)amino]-, (\alpha S)-(9CI)$  (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

RN 768363-89-9 CAPLUS

CN [1,1'-Biphenyl]-4-carboxamide, 2'-chloro-N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-90-2 CAPLUS

CN 2-Thiophenecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-

(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

RN 768363-91-3 CAPLUS

CN 2-Thiophenecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-(3-fluorophenyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-92-4 CAPLUS

CN 3-Pyrrolidinecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-oxo-1-(2-thienylmethyl)- (9CI) (CA INDEX NAME)

.RN 768363-93-5 CAPLUS

CN 3-Pyrrolidinecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-1-(2-furanylmethyl)-5-oxo-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-94-6 CAPLUS

CN 3-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-2-methyl-5-(1H-pyrrol-1-ylsulfonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-95-7 CAPLUS

CN 1H-Pyrazole-4-carboxamide, N-[(1S)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-1-phenyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 768363-96-8 CAPLUS

CN 2-Thiophenecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-(4-methylphenyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-97-9 CAPLUS

CN Benzamide, 4-(1H-benzimidazol-1-ylmethyl)-N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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CF3

RN 768363-98-0 CAPLUS

CN 1H-Pyrazole-4-carboxamide, 1-(4-chlorophenyl)-N-[(1S)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768363-99-1 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]-α-[(3-methylbenzoyl)amino]-4-(4-methylphenoxy)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-00-7 CAPLUS

CN 1H-Tetrazole-1-acetamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 768364-01-8 CAPLUS

CN 2-Thiopheneacetamide, N-[(IS)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-(3-methylphenyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Me 
$$\stackrel{H}{\longrightarrow}$$
  $\stackrel{H}{\longrightarrow}$   $\stackrel{H}{\longrightarrow}$   $\stackrel{H}{\longrightarrow}$   $\stackrel{H}{\longrightarrow}$   $\stackrel{CF_3}{\longrightarrow}$ 

RN 768364-02-9 CAPLUS

CN Pyrazolo[1,5-a]pyrimidine-6-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-2,7-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$F_3C$$
 $M_{H}$ 
 $M_$ 

RN 768364-03-0 CAPLUS

CN 3-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-2-methyl-5-(4-morpholinylsulfonyl)- (9CI) (CA INDEX NAME)

RN 768364-04-1 CAPLUS

CN 2-Thiophenecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-05-2 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-(3-methylphenyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-06-3 CAPLUS

CN 7-Benzofurancarboxamide, 2,3-dihydro-N-[(1S)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxo-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

RN 768364-07-4 CAPLUS

CN 2-Thiophenecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-(methylsulfonyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-08-5 CAPLUS

CN 4-Thiazolecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-2-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-09-6 CAPLUS

CN Benzenepropanamide,  $\alpha$ -[(3-cyanobenzoyl)amino]-N-[2-[(4-methoxyphenyl)amino]ethyl]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ NC & & & \\ & & & \\ N & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

RN 768364-10-9 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[[3-(2-methyl-4-thiazolyl)benzoyl]amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-11-0 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ [[(phenylamino)carbonyl]amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-12-1 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]- $\alpha$ -hydroxy-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 768364-13-2 CAPLUS

CN 2,1-Benzisoxazole-3-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-14-3 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-4-(difluoromethoxy)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$F_2CH$$

RN 768364-15-4 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-4-(1-methylethoxy)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-16-5 CAPLUS

CN 2-Thiophenecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-17-6 CAPLUS

CN 3-Pyridinecarboxamide, N-[(1S)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxo-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-18-7 CAPLUS

CN 4-Pyridinecarboxamide, N-[(1S)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxo-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-19-8 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-phenyl- (9CI) (CA INDEX NAME)

RN 768364-20-1 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-4-(2-methylphenoxy)-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-21-2 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-4-(5-oxazolyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-22-3 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-(4-methylphenyl)-(9CI) (CA INDEX NAME)

## Absolute stereochemistry.

RN 768364-23-4 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-3-[[(4,6-dimethyl-2-pyrimidinyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{N} \\ \text{Me} \\ \text{N} \\$$

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PAGE 1-A

CF<sub>3</sub>

RN 768364-24-5 CAPLUS

CN 4-Piperidinecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-1-(4,6-dimethyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

RN 768364-25-6 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-3-[(4,6-dimethoxy-2-pyrimidinyl)oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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RN 768364-27-8 CAPLUS

CN [1,1'-Biphenyl]-3-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-3'-methoxy- (9CI) (CA INDEX NAME)

RN 768364-28-9 CAPLUS

CN Benzeneacetamide, N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]- $\alpha$ -ethyl-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-29-0 CAPLUS

CN 2-Thiopheneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-30-3 CAPLUS

CN 3-Thiopheneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} S \\ \hline \\ M \\ \hline \\ M \\ \end{array}$$

RN 768364-31-4 CAPLUS

CN Benzenepropanamide,  $\alpha$ -[(3-bromobenzoyl)amino]-N-[2-[(4-methoxyphenyl)amino]ethyl]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-32-5 CAPLUS

CN 4-Piperidinecarboxamide, 1-acetyl-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-33-6 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-4-(4,6-dimethoxy-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

RN 768364-34-7 CAPLUS

CN 4-Piperidinecarboxamide, 1-(5-bromo-2-pyrimidinyl)-N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-35-8 CAPLUS

CN Benzenepropanamide,  $\alpha$ -[(2-cyclopenten-1-ylacetyl)amino]-N-[2-[(4-methoxyphenyl)amino]ethyl]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-36-9 CAPLUS

CN 1H-Indole-3-acetamide, N-[1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

RN 768364-37-0 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-3-(methylsulfonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-38-1 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-5-[3-(trifluoromethyl)phenyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-39-2 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-α-fluoro-(9CI) (CAINDEX NAME)

RN 768364-40-5 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-4-(trifluoromethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-42-7 CAPLUS

CN Benzenepropanamide,  $\alpha$ -[[(4-chlorophenyl)amino]carbonyl]amino]-N-[2-[(4-methoxyphenyl)amino]ethyl]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-43-8 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[[[(4-phenoxyphenyl)amino]carbonyl]amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 768364-45-0 CAPLUS

CN Benzenepropanamide,  $\alpha$ -[[[[(4-fluorophenyl)methyl]amino]carbonyl]amin o]-N-[2-[(4-methoxyphenyl)amino]ethyl]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-46-1 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-4-[(4,6-dimethyl-2-pyrimidinyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-47-2 CAPLUS

CN 3-Piperidinecarboxamide, 1-(5-bromo-2-pyrimidinyl)-N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 768364-48-3 CAPLUS

CN Benzenepropanamide,  $\alpha$ -[[(1,3-benzodioxol-5-ylamino)carbonyl]amino]-N-[2-[(4-methoxyphenyl)amino]ethyl]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-49-4 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-2,5-difluoro-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-50-7 CAPLUS

CN Benzenepropanamide,  $\alpha$ -[[[[(3-fluorophenyl)methyl]amino]carbonyl]amin o]-N-[2-[(4-methoxyphenyl)amino]ethyl]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 768364-51-8 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[[[(2-methylphenyl)amino]carbonyl]amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN .768364-52-9 CAPLUS

CN Benzenepropanamide, 4-(3,4-dichlorophenoxy)-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-53-0 CAPLUS

CN Benzeneacetamide, 3,4-dichloro-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

RN 768364-54-1 CAPLUS

CN Benzeneacetamide, 2,4-dichloro-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-55-2 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[[(1-naphthalenylamino)carbonyl]amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-56-3 CAPLUS

CN Benzenepropanamide,  $\alpha$ -[[[[2-(1,1-dimethylethyl)-6-methylphenyl]amino]carbonyl]amino]-N-[2-[(4-methoxyphenyl)amino]ethyl]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 768364-57-4 CAPLUS

CN Benzenepropanamide,  $\alpha$ -[[[(4-acetylphenyl)amino]carbonyl]amino]-N-[2-[(4-methoxyphenyl)amino]ethyl]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-58-5 CAPLUS

CN Benzenepropanamide,  $\alpha$ -[[[(3-methoxyphenyl)amino]carbonyl]amino]-N-[2-[(4-methoxyphenyl)amino]ethyl]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-59-6 CAPLUS

CN [1,1'-Biphenyl]-4-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

RN 768364-60-9 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-61-0 CAPLUS

CN Benzeneacetamide, 2-chloro-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-4-fluoro-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-62-1 CAPLUS

CN Benzamide, 2-chloro-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-3-methyl- (9CI) (CA INDEX NAME)

RN 768364-63-2 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-64-3 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-3,5-dimethyl-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-65-4 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-4-methoxy-3,5-dimethyl- (9CI) (CA INDEX NAME)

RN 768364-66-5 CAPLUS

CN Benzamide, 3-bromo-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-67-6 CAPLUS

CN 1H-Indole-2-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-5-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-68-7 CAPLUS

CN 5-Thiazolecarboxamide, 2-amino-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-

methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} H_2N & Me \\ \hline \\ S & H \\ \hline \\ O & H \\ \end{array}$$

RN 768364-69-8 CAPLUS

CN 1H-Pyrazole-4-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-1-phenyl-5-(trifluoromethyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-70-1 CAPLUS

CN 1H-Pyrazole-4-carboxamide, 1-(4-chlorophenyl)-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-(9CI) (CA INDEX NAME)

RN 768364-71-2 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-5-[3-(trifluoromethyl)phenyl](9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-72-3 CAPLUS

CN Benzamide, 3-chloro-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-73-4 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-3-(dimethylamino)- (9CI) (CA

## INDEX NAME)

Absolute stereochemistry.

$$\mathsf{Me}_2\mathsf{N} = \mathsf{N} =$$

RN 768364-74-5 CAPLUS

CN Benzamide, 3-cyano-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-75-6 CAPLUS

CN Benzamide, 4-cyano-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-76-7 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]- $\alpha$ -methyl-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

RN 768364-77-8 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-3-(2-methyl-4-thiazolyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-78-9 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-4-(1H-1,2,4-triazol-1-yl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-79-0 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-3,5-difluoro-(9CI) (CA INDEX NAME)

RN 768364-80-3 CAPLUS

CN Benzamide, N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$F_3C$$
 $H$ 
 $N$ 
 $H$ 
 $N$ 
 $H$ 
 $N$ 
 $H$ 

RN 768364-81-4 CAPLUS

Absolute stereochemistry.

RN' 768364-82-5 CAPLUS

CN Benzeneacetamide, N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]-α-methyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-83-6 CAPLUS

CN Benzamide, N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-84-7 CAPLUS

CN [1,1'-Biphenyl]-4-carboxamide, N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]- (9CI) (CA INDEX NAME)

RN 768364-85-8 CAPLUS

CN 1H-Indole-2-carboxamide, 5-chloro-N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-86-9 CAPLUS

CN 1H-Indole-2-carboxamide, N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]-5-fluoro- (9CI) (CA INDEX NAME)

RN 768364-87-0 CAPLUS

CN 5-Thiazolecarboxamide, 2-amino-N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} H_2N & Me \\ & & \\ N & S \\ & & \\ N & \\ & & \\ \end{array}$$

RN 768364-88-1 CAPLUS

CN 2-Benzofurancarboxamide, 5-chloro-N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-89-2 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]- $\alpha$ -ethyl-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

RN 768364-90-5 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]-5-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-91-6 CAPLUS

CN 6-Benzothiazolecarboxamide, N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-92-7 CAPLUS

CN Benzamide, N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]-3-(trifluoromethoxy)- (9CI) (CA INDEX NAME)

$$F_3$$
C OME

RN 768364-93-8 CAPLUS

CN Benzamide, 3-cyano-N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-94-9 CAPLUS

CN Benzamide, 4-cyano-N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-95-0 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-4-phenoxy- (9CI) (CA INDEX NAME).

Absolute stereochemistry.

RN 768364-96-1 CAPLUS

CN Benzamide, N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]-3-(2-methyl-4-thiazolyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-97-2 CAPLUS

CN Benzamide, N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]-4-(1H-1,2,4-triazol-1-yl)- (9CI) (CA INDEX NAME)

RN 768364-98-3 CAPLUS

CN [1,1'-Biphenyl]-3-carboxamide, N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768364-99-4 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-2-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-00-0 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-3,4-difluoro-(9CI) (CA

## INDEX NAME)

Absolute stereochemistry.

RN 768365-01-1 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-3-fluoro-2-methyl- (9CI) (CAINDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 768365-02-2 CAPLUS

CN Benzamide, 2-chloro-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-5-methyl- (9CI) (CA INDEX NAME)

RN 768365-03-3 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-4-fluoro-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-04-4 CAPLUS

CN 1H-Pyrazole-4-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-5-methyl-1-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-05-5 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-4-propyl- (9CI) (CA INDEX NAME)

$$\bigcap_{M \in \mathbb{N}} \bigcap_{H \in \mathbb{N}} \bigcap_{M \in \mathbb{N}} \bigcap_{$$

RN 768365-06-6 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-4-fluoro-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-07-7 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-4-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-08-8 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-2-fluoro-5-(trifluoromethyl)-(9CI) (CA INDEX NAME)

768365-09-9 CAPLUS RN

Benzamide, 3-chloro-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-CNmethoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-2-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

768365-10-2 CAPLUS RN

Benzamide, 5-chloro-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-CN methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-2-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN768365-11-3 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-5-fluoro-2-methyl- (9CI) INDEX NAME)

## Absolute stereochemistry.

RN 768365-12-4 CAPLUS

CN Cyclohexanepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[[(1-phenylcyclopropyl)carbonyl]amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\bigcap_{\text{Ph}} \bigcap_{\text{O}} \bigcap_{\text{H}} \bigcap_{\text{H}} \bigcap_{\text{OMe}}$$

RN 768365-13-5 CAPLUS

CN L-Alaninamide, N-phenylglycyl-3-cyclohexyl-N-[2-[(4-methoxyphenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-14-6 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- $\alpha$ -hydroxy-, ( $\alpha$ R)-(9CI) (CA INDEX NAME)

RN 768365-15-7 CAPLUS

CN 1H-Pyrazole-4-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-1-(4-fluorophenyl)-5-methyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-16-8 CAPLUS

CN 1H-Pyrazole-4-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-1-(4-methoxyphenyl)-5-methyl-(9CI) (CA INDEX NAME)

RN 768365-17-9 CAPLUS

CN 1H-Pyrazole-4-carboxamide, 1-(4-chlorophenyl)-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-18-0 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- $\alpha$ -ethyl-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

RN 768365-19-1 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-3-fluoro-5-(trifluoromethyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-20-4 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-2-fluoro-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-21-5 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-4-fluoro-3-methyl- (9CI) (CA INDEX NAME)

RN 768365-22-6 CAPLUS

CN 2-Furancarboxamide, 5-(4-chlorophenyl)-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-23-7 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-2-fluoro-4-(trifluoromethyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-24-8 CAPLUS

CN [1,1'-Biphenyl]-4-carboxamide, 4'-chloro-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

RN 768365-25-9 CAPLUS

CN [1,1'-Biphenyl]-4-carboxamide, 3',5'-dichloro-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-26-0 CAPLUS

CN [1,1'-Biphenyl]-4-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-3'-methoxy- (9CI) (CA INDEX NAME)

RN 768365-27-1 CAPLUS

CN [1,1'-Biphenyl]-4-carboxamide, 3'-chloro-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-28-2 CAPLUS

CN [1,1'-Biphenyl]-4-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-2'-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-29-3 CAPLUS

CN [1,1'-Biphenyl]-3-carboxamide, 4'-chloro-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-30-6 CAPLUS

CN Benzamide, 4-(1,3-benzodioxol-5-yl)-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-31-7 CAPLUS

CN 2-Furancarboxamide, 5-bromo-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-32-8 CAPLUS

CN Benzamide, 3,5-dibromo-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

# Absolute stereochemistry.

RN 768365-33-9 CAPLUS

CN Benzamide, 3,5-dichloro-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-34-0 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-3,5-dimethoxy- (9CI) (CA INDEX NAME)

RN 768365-35-1 CAPLUS

CN [1,1'-Biphenyl]-3-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-36-2 CAPLUS

CN 2-Thiophenecarboxamide, 5-bromo-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-37-3 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-4-phenoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-38-4 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-3-phenoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-39-5 CAPLUS

CN 1H-Indole-3-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-40-8 CAPLUS

CN 6-Benzothiazolecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-41-9 CAPLUS

CN 6-Benzothiazolecarboxamide, 2-amino-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

RN 768365-42-0 CAPLUS

CN 5-Thiazolecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-4-methyl-2-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-43-1 CAPLUS

CN 2-Thiophenecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-4-(4-fluorophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-44-2 CAPLUS

CN 4-Oxazolecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-2-methyl-5-(trifluoromethyl)-(9CI) (CA INDEX NAME)

# Absolute stereochemistry.

RN 768365-45-3 CAPLUS

CN 2-Thiophenecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-46-4 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- $\alpha$ -methyl-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-47-5 CAPLUS

CN 2-Furancarboxamide, 5-[2-chloro-5-(trifluoromethyl)phenyl]-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-

### (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-48-6 CAPLUS

CN 4-Piperidinecarboxamide, 1-(5-bromo-2-pyrimidinyl)-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-49-7 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]-4-[(4,6-dimethyl-2-pyrimidinyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-50-0 CAPLUS

CN 3-Piperidinecarboxamide, 1-(5-bromo-2-pyrimidinyl)-N-[(1S)-1-

(cyclohexylmethyl) -2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl](9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-51-1 CAPLUS

CN [1,1'-Biphenyl]-4-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-3'-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-52-2 CAPLUS

CN Benzamide, 3-(aminomethyl)-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-53-3 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-3-(4-morpholinylmethyl)-

### (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-54-4 CAPLUS

CN 2-Thiophenecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-(2-fluorophenyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-55-5 CAPLUS

CN Benzamide, N-[(1S)-3-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]propyl]-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-56-6 CAPLUS

CN Benzamide, N-[(1S)-4-cyclohexyl-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]butyl]-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-57-7 CAPLUS

CN Benzeneacetamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-58-8 CAPLUS

CN 2-Thiophenecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-59-9 CAPLUS

CN Benzenebutanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

768365-60-2 CAPLUS RN

2-Thiophenecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-CN (trifluoromethoxy) phenyl] amino] ethyl] amino] ethyl] -5-[4-(trifluoromethoxy)phenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

$$F_3C$$

PAGE 1-B

 $\sim$  CF3

RN 768365-61-3 CAPLUS

CNBenzamide, N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-4phenyl-3-butenyl]-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 768365-62-4 CAPLUS

2-Thiophenecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-CN (trifluoromethoxy) phenyl] amino] ethyl] amino] ethyl] -5-[3-(trifluoromethoxy)phenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$F_3C$$

PAGE 1-B

PAGE 1-A

 $\sim$  CF3

Absolute stereochemistry.

RN 768365-64-6 CAPLUS

CN Benzeneacetamide, 4-methoxy-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-66-8 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-67-9 CAPLUS

CN Benzeneacetamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-2-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 768365-68-0 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-[4-(trifluoromethoxy)phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$F_3C$$

PAGE 1-B

 $\sim$  CF3

RN 768365-69-1 CAPLUS

CN Benzeneacetamide, 2-chloro-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]- (9CI) (CA INDEX NAME)

RN 768365-70-4 CAPLUS

CN Benzeneacetamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Ph-CH}_2\text{-O} \\ \\ \text{O} \\ \\ \text{O$$

RN 768365-71-5 CAPLUS

CN 1-Naphthaleneacetamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]- (9CI) (CA INDEX NAME)

RN 768365-72-6 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-73-7 CAPLUS

CN Benzeneacetamide, N-[2-[(4-methoxyphenyl)amino]ethyl]-2-methyl- $\alpha$ -[(3-methylbenzoyl)amino]- (9CI) (CA INDEX NAME)

RN 768365-74-8 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]-4-(1H-1,2,4-triazol-1-yl)- (9CI) (CA INDEX NAME)

RN 768365-75-9 CAPLUS

CN Benzeneacetamide, 2,4-dichloro-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 768365-76-0 CAPLUS

CN Benzeneacetamide, 2,3-dichloro-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]- (9CI) (CA INDEX NAME)

RN 768365-77-1 CAPLUS

CN Benzeneacetamide, N-[2-[(4-methoxyphenyl)amino]ethyl]-2,4-dimethyl- $\alpha$ -[(3-methylbenzoyl)amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{NH-CH}_2\text{-CH}_2\text{-NH-C} \\ \text{CH-NH-C} \\ \text{O} \\ \end{array}$$

RN 768365-78-2 CAPLUS

CN Benzeneacetamide, 2,4-dimethoxy-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]- (9CI) (CA INDEX NAME)

RN 768365-79-3 · CAPLUS

CN 2-Thiopheneacetamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]- (9CI) (CA INDEX NAME)

RN 768365-80-6 CAPLUS

CN Benzeneacetamide, 4-fluoro-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]- (9CI) (CA INDEX NAME)

RN 768365-81-7 CAPLUS

CN Benzenepropanamide, 4-hydroxy-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-82-8 CAPLUS

CN Benzenepropanamide, 2,4-dichloro-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-83-9 CAPLUS

CN Benzenepropanamide, 3,5-difluoro-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 768365-84-0 CAPLUS

CN Benzenepropanamide, 3,4-dichloro-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-85-1 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-86-2 CAPLUS

CN Benzenepropanamide, 4-(acetylamino)-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 768365-87-3 CAPLUS

CN [1,1'-Biphenyl]-4-carboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-88-4 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]-4-methyl- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-89-5 CAPLUS

CN Benzenepropanamide, 3-fluoro-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 768365-90-8 CAPLUS

CN Benzenepropanamide, 3,4-difluoro-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-91-9 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]-3-methyl- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-92-0 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-2-(trifluoromethyl)-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

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768365-93-1P 768365-94-2P 768365-95-3P
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     768365-99-7P 768366-00-3P 768366-01-4P
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     768366-77-4P 768366-78-5P 768368-72-5P
     768368-73-6P
     RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (inhibitors of cathepsin S for use in disease treatment)
RN
     768365-93-1 CAPLUS
CN
     Benzenepropanamide, 4-cyano-N-[2-[(4-methoxyphenyl)amino]ethyl]-\alpha-
     [(3-methylbenzoyl)amino]-, (\alphaS)- (9CI) (CA INDEX NAME)
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RN 768365-94-2 CAPLUS

CN Benzenepropanamide, 4-bromo-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-95-3 CAPLUS

CN Benzenepropanamide, 4-iodo-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-96-4 CAPLUS

CN Benzenepropanamide, 4-chloro-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 768365-97-5 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-4-nitro-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & & \\$$

RN 768365-98-6 CAPLUS

CN Benzenepropanamide, 4-fluoro-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ [(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768365-99-7 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-5-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 768366-00-3 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-4-(phenylmethoxy)-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-01-4 CAPLUS

CN Benzenepropanamide, 4-[(2,6-dichlorophenyl)methoxy]-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-02-5 CAPLUS

CN Benzenepropanamide, 4-methoxy-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 768366-03-6 CAPLUS

CN 5-Thiazolecarboxamide, 2-amino-N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-04-7 CAPLUS

CN 2-Furancarboxamide, 5-[2-chloro-5-(trifluoromethyl)phenyl]-N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-05-8 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-3-(trifluoromethyl)-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 768366-06-9 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-4-(trifluoromethyl)-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-07-0 CAPLUS

CN Benzamide, N-[(1S)-2-[[2-[(4-methoxyphenyl)amino]ethyl]amino]-2-oxo-1-[(phenylmethoxy)methyl]ethyl]-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-08-1 CAPLUS

CN Benzenepropanamide, 4-(1,1-dimethylethyl)-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

RN 768366-09-2 CAPLUS

CN 1H-Indole-3-propanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-10-5 CAPLUS

CN 1-Naphthalenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-11-6 CAPLUS

CN Benzamide, N-[(1S,2R)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-2-(phenylmethoxy)propyl]-3-methyl- (9CI) (CA INDEX NAME)

RN 768366-12-7 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-3-fluoro-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-13-8 CAPLUS

CN 2-Naphthalenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-14-9 CAPLUS

CN 3-Pyridinepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 768366-15-0 CAPLUS

CN 4-Pyridinepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-16-1 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-17-2 CAPLUS

CN 1H-1,2,4-Triazole-1-acetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

RN 768366-18-3 CAPLUS

CN Benzenebutanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-4-nitro-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-19-4 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-4-(3-methylphenoxy)-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-20-7 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\beta$ -methyl- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ R, $\beta$ S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 768366-21-8 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\beta$ -methyl- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ R, $\beta$ R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 768366-22-9 CAPLUS

CN [1,1'-Biphenyl]-4-propanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-23-0 CAPLUS

CN [1,1'-Biphenyl]-4-propanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-3'-nitro-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 768366-24-1 CAPLUS

CN 3-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-25-2 CAPLUS

CN [1,1'-Biphenyl]-4-propanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-2'-nitro-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-26-3 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-4-(3-pyridinyl)-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 768366-27-4 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-4-(3-thienyl)-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-28-5 CAPLUS

CN [1,1'-Biphenyl]-4-propanamide, 4'-cyano-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-29-6 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-4-(4-pyridinyl)-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 768366-30-9 CAPLUS

CN [1,1'-Biphenyl]-4-propanamide, 4'-chloro-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-31-0 CAPLUS

CN [1,1'-Biphenyl]-4-propanamide, 2',3'-dimethoxy-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-32-1 CAPLUS

CN [1,1'-Biphenyl]-4-propanamide, 3'-amino-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-

# Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 768366-33-2 CAPLUS

CN [1,1'-Biphenyl]-4-propanamide, 3',4'-dimethoxy-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-34-3 CAPLUS

CN [1,1'-Biphenyl]-4-propanamide, 4'-(hydroxymethyl)-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

RN 768366-35-4 CAPLUS CN [1,1'-Biphenyl]-4-propanamide, 5'-fluoro-2'-methoxy-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-36-5 CAPLUS
CN [1,1'-Biphenyl]-4-propanamide, 3'-(hydroxymethyl)-N-[2-[(4-methoxyphenyl)amino]ethyl]-α-[(3-methylbenzoyl)amino]-, (αS)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-37-6 CAPLUS CN [1,1'-Biphenyl]-4-propanamide, 2',5'-dimethoxy-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-

(9CI) (CA INDEX NAME)

RN 768366-38-7 CAPLUS

CN [1,1'-Biphenyl]-4-propanamide, 2',5'-dichloro-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-39-8 CAPLUS

CN [1,1'-Biphenyl]-4-propanamide, 4'-(dimethylamino)-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ &$$

RN 768366-40-1 CAPLUS

CN [1,1'-Biphenyl]-4-propanamide, 2'-acetyl-N-[2-[(4-

methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-41-2 CAPLUS

CN [1,1'-Biphenyl]-4-propanamide, 4'-hydroxy-N-[2-[(4-methoxyphenyl)amino]ethyl]-α-[(3-methylbenzoyl)amino]-, (αS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-42-3 CAPLUS

CN [1,1'-Biphenyl]-4-propanamide, 3'-acetyl-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

RN 768366-43-4 CAPLUS

CN Benzenepropanamide,  $4-(2,4-\text{dimethoxy-5-pyrimidiny1})-N-[2-[(4-\text{methoxypheny1})amino]ethyl]-<math>\alpha-[(3-\text{methylbenzoy1})amino]-, (\alpha S)-(9CI)$  (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-44-5 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]-4-(6-methoxy-3-pyridinyl)- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-45-6 CAPLUS

CN 2-Thiophenecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-5-(methylsulfonyl)- (9CI) (CFINDEX NAME)

RN 768366-46-7 CAPLUS CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- $\alpha$ -methyl-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-47-8 CAPLUS

CN 4-Pyridazinecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-48-9 CAPLUS

CN Cyclohexanepropanamide,  $\alpha$ -[(cyclopropylcarbonyl)amino]-N-[2-[(4-fluorophenyl)amino]ethyl]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-49-0 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-4-[(methylsulfonyl)amino]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-50-3 CAPLUS

CN Benzenepropanamide, 4-(4-chlorophenoxy)-N-[2-[(4-methoxyphenyl)amino]ethyl]-α-[(3-methylbenzoyl)amino]-, (αS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-51-4 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-4-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN 768366-52-5 CAPLUS

CN Benzeneacetamide, 3-chloro-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

RN 768366-53-6 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-54-7 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-55-8 CAPLUS

CN Benzeneacetamide, 4-chloro-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

RN 768366-56-9 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-2-fluoro-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-57-0 CAPLUS

CN [1,1'-Biphenyl]-4-acetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-58-1 CAPLUS

'CN [1,1'-Biphenyl]-4-acetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-3-fluoro-α-methyl- (9CI) (CA INDEX NAME)

RN 768366-59-2 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- $\alpha$ ,4-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} Me \\ \hline \\ Me \\ \hline \\ Me \\ O \end{array}$$

RN 768366-60-5 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-4-fluoro- $\alpha$ -methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN '768366-61-6 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-4-hydroxy- $\alpha$ -methyl-(9CI) (CA INDEX NAME)

RN 768366-62-7 CAPLUS

CN Benzeneacetamide, 4-chloro-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- $\alpha$ -methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-63-8 CAPLUS

CN Benzamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-4-(methylsulfonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN 768366-64-9 CAPLUS

CN 4-Thiazolecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

RN 768366-65-0 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- $\alpha$ -methyl-, ( $\alpha$ R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-66-1 CAPLUS

CN Benzamide, 4-cyano-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-67-2 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- $\alpha$ -hydroxy-, ( $\alpha$ R)-(9CI) (CA INDEX NAME)

RN 768366-68-3 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- $\alpha$ -ethyl-, ( $\alpha$ R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-69-4 CAPLUS

CN Cyclohexanepropanamide, N-[2-[(4-fluorophenyl)amino]ethyl]- $\alpha$ -[[(1-phenylcyclopropyl)carbonyl]amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-70-7 CAPLUS

CN Benzamide, 3-cyano-N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

RN 768366-71-8 CAPLUS

CN 2-Furancarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-5-(4-fluorophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-72-9 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-73-0 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 768366-74-1 CAPLUS

CN Benzeneacetamide, N-[(1S)-1-(cyclohexylmethyl)-2-[[2-[(4-fluorophenyl)amino]ethyl]amino]-2-oxoethyl]-4-(methylsulfonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-75-2 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-4-phenoxy-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-76-3 CAPLUS

CN Benzenepropanamide, 4-(4-methoxyphenoxy)-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

RN 768366-77-4 CAPLUS

CN Benzenepropanamide, 4-(3-chlorophenoxy)-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-78-5 CAPLUS

CN Benzenepropanamide, 4-(3,5-dimethylphenoxy)-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768368-72-5 CAPLUS

CN 3-Thiophenecarboxamide, N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768368-73-6 CAPLUS

CN [1,1'-Biphenyl]-3-carboxamide, 2'-chloro-N-[(1S)-1-(cyclohexylmethyl)-2-oxo-2-[[2-[[4-(trifluoromethoxy)phenyl]amino]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 768364-11-0DP, resin conjugates 768366-90-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(inhibitors of cathepsin S for use in disease treatment)

RN 768364-11-0 CAPLUS

CN Benzenepropanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(phenylamino)carbonyl]amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-90-1 CAPLUS

CN Benzenepropanamide, 4-(1,1-dimethylethoxy)-N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & & \\$$

#### IT 768366-79-6P 768366-80-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (inhibitors of cathepsin S for use in disease treatment)

RN 768366-79-6 CAPLUS

CN Benzenepropanamide, α-[(3-methoxybenzoyl)amino]-N-[2-[(4-methoxyphenyl)amino]ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 768366-80-9 CAPLUS

CN Benzenepentanamide, N-[2-[(4-methoxyphenyl)amino]ethyl]- $\alpha$ -[(3-methylbenzoyl)amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

- L4 ANSWER 4 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 2004:781509 CAPLUS
- DN 142:34412
- TI Differences in substrate specificities between cysteine protease CPB isoforms of Leishmania mexicana are mediated by a few amino acid changes
- AU Juliano, Maria A.; Brooks, Darren R.; Selzer, Paul M.; Pandolfo, Hector L.; Judice, Wagner A. S.; Juliano, Luiz; Meldal, Morten; Sanderson, Sanya J.; Mottram, Jeremy C.; Coombs, Graham H.
- CS Department of Biophysics, Escola Paulista de Medicina, Universidade Federal de Sao Paulo, Brazil

SO European Journal of Biochemistry (2004), 271(18), 3704-3714 CODEN: EJBCAI; ISSN: 0014-2956

PB Blackwell Publishing Ltd.

DT Journal

LA English

The CPB genes of the protozoan parasite Leishmania mexicana encode AB stage-regulated cathepsin L-like cysteine proteases that are important virulence factors and are in a tandem array of 19 genes. In this study, we have compared the substrate preferences of two CPB isoforms, CPB2.8 and CPB3, and a H84Y mutant of the latter enzyme, to analyze the roles played by the few amino acid differences between the isoenzymes in determining substrate specificity. CPB3 differs from CPB2.8 at just three residues (N60D, D61N and D64S) in the mature domain. The H84Y mutation mimics an addnl. change present in another isoenzyme, CPB18. The active recombinant CPB isoenzymes and mutant were produced using Escherichia coli and the S1-S3 and S1'-S3' subsite specificities determined using a series of fluorogenic peptide derivs. in which substitutions were made on positions P3 to P3' by natural amino acids. Carboxydipeptidase activities of CPB3 and H84Y were also observed using the peptide Abz-FRAK(Dnp)-OH and some of its analogs. The kinetic parameters of hydrolysis by CPB3, H84Y and CPB2.8 of the synthetic substrates indicates that the specificity of S3 to S3' subsites is influenced greatly by the modifications at amino acids 60, 61, 64 and 84. Particularly noteworthy was the large preference for Pro in the P2' position for the hydrolytic activity of CPB3, which may be relevant to a role in the activation mechanism of the L. mexicana CPBs.

IT 364630-60-4 364630-61-5

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(S3' subsite specificity; differences in substrate specificities between cysteine proteinase CPB isoforms of Leishmania mexicana are mediated by a few amino acid changes)

RN 364630-60-4 CAPLUS

CN L-Glutamamide, N2-(2-aminobenzoyl)-L-lysyl-L-leucyl-L-arginyl-L-phenylalanyl-L-seryl-L-prolyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 364630-61-5 CAPLUS

CN L-Glutamamide, N2-(2-aminobenzoyl)-L-lysyl-L-leucyl-L-arginyl-L-phenylalanyl-L-seryl-L-phenylalanyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:511072 CAPLUS

DN 142:214127

TI Fluorogenic peptide substrates for carboxydipeptidase activity of cathepsin B

- AU Stachowiak, Krystyna; Tokmina, Monika; Karpinska, Anna; Sosnowska, Renata; Wiczk, Wieslaw
- CS Faculty of Chemistry, University of Gdansk, Gdansk, 80-952, Pol.
- SO Acta Biochimica Polonica (2004), 51(1), 81-92 CODEN: ABPLAF; ISSN: 0001-527X
- PB Polish Biochemical Society
- DT Journal
- LA English
- Cathepsin B is a lysosomal cysteine protease exhibiting mainly dipeptidyl AB carboxypeptidase activity, which decreases dramatically above pH 5.5, when the enzyme starts acting as an endopeptidase. Since the common cathepsin B assays are performed at pH 6 and do not distinguish between these activities, we synthesized a series of peptide substrates specifically designed for the carboxydipeptidase activity of cathepsin B. The amino-acid sequences of the P5-P1 part of these substrates were based on the binding fragments of cystatin C and cystatin SA, the natural reversible inhibitors of papain-like cysteine protease. The sequences of the P'1-P'2 dipeptide fragments of the substrates were chosen on the basis of the specificity of the S'1-S'2 sites of the cathepsin B catalytic cleft. The rates of hydrolysis by cathepsin B and papain, the archetypal cysteine protease, were monitored by a continuous fluorescence assay based on internal resonance energy transfer from an Edans to a Dabcyl group. The fluorescence energy donor and acceptor were attached to the C- and the N-terminal amino-acid residues, resp. The kinetics of hydrolysis followed the Michaelis-menten model. Out of all the examined peptides Dabcyl-R-L-V-G-F-E(Edans) turned out to be very good substrate for both papain and cathepsin B at both pH 6 and pH 5. The replacement of Glu by Asp turned this peptide into an exclusive substrate for cathepsin B not hydrolyzed by papain. The substitution of Phe by Nal in the original substrate caused an increase of the specificity constant for cathepsin B at pH 5, and a significant decrease at pH 6. The results of kinetic studies also suggest that Arg in position P4 is not important for the exopeptidase activity of cathepsin B, and that introducing Glu in place of Val in position P2 causes an increase of the substrate preference towards this activity.
- IT 843640-37-9 843640-38-0 843640-39-1 843640-40-4 843640-41-5 843640-42-6 843640-43-7 843640-44-8 843640-45-9

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(kinetic studies of fluorogenic peptide substrates for carboxydipeptidase activity of cathepsin B)

RN 843640-37-9 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 843640-38-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

\_\_\_NH2

RN 843640-39-1 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 843640-40-4 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 843640-41-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 843640-42-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 843640-43-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 843640-44-8 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 843640-45-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry. Double bond geometry unknown.

PAGE 1-A

### RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 6 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 2004:488023 CAPLUS
- DN 142:129543
- TI Design and use of highly specific substrates of neutrophil elastase and proteinase 3
- AU Korkmaz, Brice; Attucci, Sylvie; Moreau, Thierry; Godat, Emmanuel; Juliano, Luiz; Gauthier, Francis
- CS INSERM U618, Proteases et Vectorisation Pulmonaires, University Francois Rabelais, Tours, Fr.
- SO American Journal of Respiratory Cell and Molecular Biology (2004), 30(6), 801-807
  CODEN: AJRBEL; ISSN: 1044-1549
- PB American Thoracic Society
- DT Journal
- LA English
- We have exploited differences in the structures of S2' subsites of AB proteinase 3 (Pr3) and human neutrophil elastase (HNE) to prepare new fluorogenic substrates specific for each of these proteases. The pos. charged residue at position 143 in Pr3 prevents it from accommodating an arginyl residue at S2' and improves the binding of P2' aspartyl-containing substrates, as judged by the decreased Km. As a result, the kcat/Km for Abz-VADCADQ-EDDnp is over 500 times greater for Pr3 than for HNE, and that for Abz-APEEIMRRQ-EDDnp is over 500 times greater for HNE than for Pr3. This allows each protease activity to be measured in the presence of a large excess of the other, as might occur in vivo. Placing a prolyl residue in position P2' greatly impaired substrate binding to both HNE and Pr3, which further emphasizes the importance of S' subsites in these proteases. HNE and Pr3 activities were measured with these substrates at the surface of fixed polymorphonuclear leukocytes (PMNs) before and after activation. This demonstrated that their active site remains accessible when they are exposed to the cell surface. Both membrane-bound proteases were strongly inhibited by low Mr serine protease inhibitors, but only

partially by inhibitors of larger Mr such as  $\alpha 1$ -protease inhibitor, the main physiol. inhibitor in lung secretions. Most of membrane-bound HNE and Pr3 can be released from the membrane surface of fixed cells by a buffer containing detergent, suggesting that hydrophobic interactions are involved in membrane binding.

IT 824405-65-4 824405-66-5

RL: BSU (Biological study, unclassified); BIOL (Biological study) (design and use of highly specific substrates of neutrophil elastase and proteinase 3)

RN 824405-65-4 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)-L-alanyl-L-prolyl-L- $\alpha$ -glutamyl-L- $\alpha$ -glutamyl-L-isoleucyl-L-methionyl-L- $\alpha$ -aspartyl-L-tyrosyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RN 824405-66-5 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)-L-alanyl-L-prolyl-L- $\alpha$ -glutamyl-L-  $\alpha$ -glutamyl-L-isoleucyl-L-methionyl-L- $\alpha$ -aspartyl-L-arginyl-L-tyrosyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

$$CO_2H$$
 $CO_2H$ 
 $NO_2$ 
 $NO_2$ 
 $NO_2$ 
 $NO_2$ 
 $NO_2$ 
 $NO_2$ 

## RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:409172 CAPLUS

DN 141:116438

TI Aminoacyl-analogues of mitoxantrone as novel DNA-damaging cytotoxic agents

AU Zagotto, Giuseppe; Sissi, Claudia; Gatto, Barbara; Palumbo, Manlio

CS Department of Pharmaceutical Sciences, University of Padova, Padua, 35131, Italy

SO ARKIVOC (Gainesville, FL, United States) (2004), (5), 204-218 CODEN: AGFUAR

URL: http://www.arkat-usa.org/ark/journal/2004/Tortorella/Vt-1019L/1019L.pdf

PB Arkat USA Inc.

DT Journal; (online computer file)

LA English

OS CASREACT 141:116438

AB Anthracenedione derivs. are widely used structures to target DNA in chemotherapy. One of the major problem related to their use is their lack of sequence selectivity along the genome. With the aim of favoring recognition of selected DNA sequences, we synthesized four novel aminoacyl derivs. Two side chains carrying amino acid residues different for charge and chirality have been introduced at positions 1 and 4 of 5,8-dihydroxyanthracene-9,10-dione. An aminoethylamino spacer was

inserted between the planar ring system and the selected amino acid residues. Investigations in DNA binding properties of these new derivs. showed a large modulation of the drugs affinities for the nucleic acid depending upon the charge of the amino acid used but irresp. of its chirality. However, as shown by topoisomerase II poisoning, prominent DNA-binding properties did not grant superior topoisomerase inhibition due mainly to template effect. In turn, amino acid chirality plays a critical role in the in vitro cytotoxicity, L enantiomers being much more effective than D enantiomers. These findings suggest that conjugation of the anthracenedione moiety to amino acids/peptides can be a valuable tool to selectively target cancer cells.

IT 723302-14-5P 723302-15-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(aminoacyl-analogs of mitoxantrone as novel DNA-damaging cytotoxic agents)

RN 723302-14-5 CAPLUS

CN Carbamic acid, [(9,10-dihydro-5,8-dihydroxy-9,10-dioxo-1,4-anthracenediyl)bis[imino-2,1-ethanediylimino[(1S)-1-[4-[[(1,1-dimethylethoxy)carbonyl]amino]butyl]-2-oxo-2,1-ethanediyl]]]bis-,bis(9H-fluoren-9-ylmethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 3-A

RN 723302-15-6 CAPLUS

CN Carbamic acid, [(9,10-dihydro-5,8-dihydroxy-9,10-dioxo-1,4-anthracenediyl)bis[imino-2,1-ethanediylimino[(1R)-1-[4-[[(1,1-dimethylethoxy)carbonyl]amino]butyl]-2-oxo-2,1-ethanediyl]]bis-, bis(9H-fluoren-9-ylmethyl) ester (9CI) (CA INDEX NAME)

PAGE 2-A

# RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:389415 CAPLUS

DN 141:152878

TI On the Sequential Determinants of Calpain Cleavage

AU Tompa, Peter; Buzder-Lantos, Peter; Tantos, Agnes; Farkas, Attila; Szilagyi, Andras; Banoczi, Zoltan; Hudecz, Ferenc; Friedrich, Peter

CS Biological Research Center, Institute of Enzymology, Hungarian Academy of Sciences, Budapest, H-1528, Hung.

SO Journal of Biological Chemistry (2004), 279(20), 20775-20785 CODEN: JBCHA3; ISSN: 0021-9258

PB American Society for Biochemistry and Molecular Biology

DT Journal

LA English

AB The structural clues of substrate recognition by calpain are incompletely understood. In this study, 106 cleavage sites in substrate proteins compiled from the literature have been analyzed to dissect the signal for calpain cleavage and also to enable the design of an ideal calpain substrate and interfere with calpain action via site-directed mutagenesis. In general, our data underline the importance of the primary structure of the substrate around the scissile bond in the recognition process. Significant amino acid preferences were found to extend over 11 residues around the scissile bond, from P4 to P7'. In compliance with earlier data, preferred residues in the P2 position are Leu, Thr, and Val, and in P1 Lys, Tyr, and Arq. In position P1', small hydrophilic residues, Ser and to a lesser extent Thr and Ala, occur most often. Pro dominates the region flanking the P2-P1' segment, i.e. positions P3 and P2'-P4'; most notable is its occurrence 5.59 times above chance in P3'. Intriguingly, the segment C-terminal to the cleavage site resembles the consensus inhibitory region of calpastatin, the specific inhibitor of the enzyme. Further, the position of the scissile bond correlates with certain sequential attributes, such as secondary structure and PEST score, which, along with the amino acid preferences, suggests that calpain cleaves within rather disordered segments of proteins. The amino acid preferences were confirmed by site-directed mutagenesis of the autolysis sites of Drosophila calpain B; when amino acids at key positions were changed to less preferred ones, autolytic cleavage shifted to other, adjacent sites. Based on these preferences, a new fluorogenic calpain substrate, DABCYLTPLKSPPPSPR-EDANS, was designed and synthesized. In the case of μ- and m-calpain, this substrate is kinetically superior to com. available ones, and it can be used for the in vivo assessment of the activity of these ubiquitous mammalian calpains.

IT 728005-83-2P

RL: BSU (Biological study, unclassified); PNU (Preparation, unclassified); PRP (Properties); BIOL (Biological study); PREP (Preparation) (engineering of most preferred fluorogenic calpain substrate)

RN 728005-83-2 CAPLUS

CN L-Argininamide, N-[4-[[4-(dimethylamino)phenyl]azo]benzoyl]-L-threonyl-L-prolyl-L-leucyl-L-lysyl-L-seryl-L-prolyl-L-prolyl-L-prolyl-L-seryl-L-

Absolute stereochemistry.

Double bond geometry unknown.

PAGE 1-A

PAGE 1-B

PAGE 2-C

RE.CNT 86 THERE ARE 86 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 9 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 2003:799807 CAPLUS
- DN 140:141610
- TI Probing cathepsin K activity with a selective substrate spanning its active site
- AU Lecaille, Fabien; Weidauer, Enrico; Juliano, Maria A.; Bromme, Dieter; Lalmanach, Gilles
- CS Faculte de Medecine, Laboratoire d'Enzymologie et Chimie des Proteines, INSERM EMI-U 00-10 'Proteases et Vectorisation', Universite Francois Rabelais, Tours, F-37032, Fr.
- SO Biochemical Journal (2003), 375(2), 307-312 CODEN: BIJOAK; ISSN: 0264-6021
- PB Portland Press Ltd.
- DT Journal
- LA English
- AB The limited availability of highly selective cathepsin substrates seriously impairs studies designed to monitor individual cathepsin activities in biol samples. Among mammalian cysteine proteases,

cathepsin K has a unique preference for a proline residue at P2, the primary determinant of its substrate specificity. Interestingly, congopain from Trypanosoma congolense also accommodates a proline residue in its S2 subsite. Anal. of a congopain model showed that amino acids forming its S2 subsite are identical with those of cathepsin K, except Leu67 which is replaced by a tyrosine residue in cathepsin K. Furthermore, amino acid residues of the congopain S2' binding pocket, which accepts a proline residue, are strictly identical with those of cathepsin K. Abz-HPGGPQ-EDN2ph [where Abz represents o-aminobenzoic acid and EDN2ph (=EDDnp) represents N - (2,4-dinitrophenyl) - ethylenediamine], a substrate initially developed for trypanosomal enzymes, was efficiently cleaved at the Gly-Gly bond by cathepsin K (k cat/ K m=426000 M-1·s-1). On the other hand, Abz-HPGGPQ-EDN2ph was resistant to hydrolysis by cathepsins B, F, H, L, S and V (20 nM enzyme concentration) and

the

Y67L (Tyr67 Leu)/L205A cathepsin K mutant (20 nM), but still acted as a competitive inhibitor. Taken together, the selectivity of Abz-HPGGPQ-EDN2ph to cathepsin K primarily depends on the S2 and S2' subsite specificities of cathepsin K and the ionization state of histidine at P3. Whereas Abz-HPGGPQ-EDN2ph was hydrolyzed by wild-type mouse fibroblast lysates, its hydrolysis was completely abolished in the cathepsin K-deficient samples, indicating that Abz-HPGGPQ-EDN2ph can be used to monitor selectively cathepsin K activity in physiol. fluids and cell lysates.

IT 221055-89-6

RL: BSU (Biological study, unclassified); BIOL (Biological study) (cathepsin K activity with a selective substrate spanning its active site)

RN 221055-89-6 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)-L-histidyl-L-prolylglycylglycyl-L-prolyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

## RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:746476 CAPLUS

DN 140:35040

TI Adsorption isotherms and retention behavior of 1,1'-bis(2-naphthol) on CHIRIS AD1 and CHIRIS AD2 columns

AU Skavrada, Michal; Jandera, Pavel; Cherrak, Djamel E.; Aced, Ahmed; Guiochon, G.

CS Department of Analytical Chemistry, University of Pardubice, Pardubice, CZ 532 10, Czech Rep.

SO Journal of Chromatography, A (2003), 1016(2), 143-154 CODEN: JCRAEY; ISSN: 0021-9673

PB Elsevier Science B.V.

DT Journal

LA English

AB The separation of the atropoisomers of 1,1'-bis(2-naphthol) was studied on CHIRIS AD1 and CHIRIS AD2, two Pirkle-type chiral stationary phases. Satisfactory selectivity was found only on CHIRIS AD2. The ternary mobile phases comprised hexane, dichloromethane and methanol. The effects of their composition and of the temperature on the retention under anal.

conditions and

on the single-component and competitive isotherms were studied. The retention of the R- and S-isomers on CHIRIS AD1 and CHIRIS AD2 is controlled by the enthalpic contribution to adsorption, but the effect of the mobile phase on the retention should be attributed mainly to the entropic contribution. The adsorption of the less retained R-isomer is controlled by the achiral interactions, which are the same as for the S-isomer. The single-component and competitive isotherms of the R- and S-isomers are adequately described by the sum of a Langmuir term for the achiral contribution to adsorption and a linear-term characterizing the selective or chiral adsorption of the S-isomer in the concentration range exptl.

available, i.e. within the solubility limit of 1,1'-bis(2-naphthol).

IT 634602-72-5D, silica gel supported 634602-73-6D, silica gel supported

RL: ARU (Analytical role, unclassified); NUU (Other use, unclassified); ANST (Analytical study); USES (Uses)

(chiral selector; adsorption isotherms and retention behavior of bisnaphthol on CHIRIS AD1 and CHIRIS AD2 columns)

RN 634602-72-5 CAPLUS

CN Benzeneacetamide, N,N'-[[4-chloro-2,6-dicyano-5-[[3-(trihydroxysilyl)propyl]amino]-1,3-phenylene]bis(imino-2,1-ethanediyl)]bis[ $\alpha$ -[(3,5-dinitrobenzoyl)amino]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RN 634602-73-6 CAPLUS

CN Benzamide, N,N'-[[4-chloro-2,6-dicyano-5-[[3-(trihydroxysilyl)propyl]amino ]-1,3-phenylene]bis[imino-2,1-ethanediylimino[1-(2-methylpropyl)-2-oxo-2,1-ethanediyl]]]bis[3,5-dinitro-(9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:577343 CAPLUS

DN 140:266600

TI S3 to S3' subsite specificity of recombinant human cathepsin K and development of selective internally quenched fluorescent substrates

AU Alves, Marcio F. M.; Puzer, Luciano; Cotrin, Simone S.; Juliano, Maria Aparecida; Juliano, Luiz; Broemme, Dieter; Carmona, Adriana K.

CS Department of Biophysics, Escola Paulista de Medicina, UNIFESP, Sao Paulo, 04044-020, Brazil

SO Biochemical Journal (2003), 373(3), 981-986 CODEN: BIJOAK; ISSN: 0264-6021

PB Portland Press Ltd.

DT Journal

LA English

We have systematically examined the S3 to S3' subsite substrate specificity AΒ requirements of cathepsin K using internally quenched fluorescent peptides derived from the lead sequence Abz-KLRFSKQ-EDDnp [where Abz is o -aminobenzoic acid and EDDnp is N-(2,4-dinitrophenyl)ethylenediamine]. assayed six series of peptides, in which each position except Gln was substituted with various natural amino acids. The results indicated that the S3-S1 subsite requirements are more restricted than those of S1'-S3'. Cathepsin K preferentially accommodates hydrophobic amino acids with aliphatic side chains (Leu, Ile and Val) in the S2 site. Modifications at P1 residues also have a large influence on cathepsin K activity. charged residues (Arg and Lys) represent the best accepted amino acids in this position, although a particular preference for Gly was found as well. Subsite S3 accepted preferentially basic amino acids such as Lys and Arg. A broad range of amino acids was accommodated in the remaining subsites. We further explored the acceptance of a Pro residue in the P2 position by cathepsin K in order to develop specific substrates for the enzyme. series of peptides with the general sequences Abz-KXPGSKQ-EDDnp and Abz-KPXGSKQ-EDDnp (where X denotes the position of the amino acid that is altered) were synthesized. The substrates Abz-KPRGSKQ-EDDnp and Abz-KKPGSKQ-EDDnp were cleaved by cathepsin K at the Arg-Gly and Gly-Ser bonds resp., and have been shown to be specific for cathepsin K when compared with other lysosomal cysteine proteases such as cathepsins L and B and with the aspartyl protease cathepsin D.

IT 364630-60-4 364630-61-5

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(S3 to S3' subsite specificity of recombinant human cathepsin K and development of selective internally quenched fluorescent substrates)

RN 364630-60-4 CAPLUS CN L-Glutamamide, N2-(

L-Glutamamide, N2-(2-aminobenzoyl)-L-lysyl-L-leucyl-L-arginyl-L-phenylalanyl-L-seryl-L-prolyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]-(9CI) (CA INDEX NAME)

RN 364630-61-5 CAPLUS

CN L-Glutamamide, N2-(2-aminobenzoyl)-L-lysyl-L-leucyl-L-arginyl-L-phenylalanyl-L-seryl-L-phenylalanyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN AN 2003:577328 CAPLUS

DN 140:266599

- TI Subsite specificity (S3, S2, S1', S2' and S3') of oligopeptidase B from Trypanosoma cruzi and Trypanosoma brucei using fluorescent quenched peptides: comparative study and identification of specific carboxypeptidase activity
- AU Hemerly, Jefferson P.; Oliveira, Vitor; Del Nery, Elaine; Morty, Rory E.; Andrews, Norma W.; Juliano, Maria A.; Juliano, Luiz
- CS Department of Biophysics, Escola Paulista de Medicina, Sao Paulo, 04044-020, Brazil
- SO Biochemical Journal (2003), 373(3), 933-939 CODEN: BIJOAK; ISSN: 0264-6021
- PB Portland Press Ltd.
- DT Journal
- LA English
- AB We characterized the extended substrate binding site of recombinant oligopeptidase B enzymes from Trypanosoma cruzi (Tc-OP) and Trypanosoma brucei (Tb-OP), evaluating the specificity of their S3, S2, S1', S2' and S3' subsites. Five series of internally quenched fluorescent peptides based on the substrate Abz-AGGRGAQ-EDDnp [where Abz is o -aminobenzoic acid and EDDnp is N - (2,4-dinitrophenyl) ethylenediamine) were designed to contain amino acid residues with side chains of a min. size, and each residue position of this substrate was modified. Synthetic peptides of different lengths derived from the human kiningeen sequence were also examined, and peptides of up to 17 amino acids were found to be hydrolyzed by Tc-OP and Tb-OP. These two oligopeptidases were essentially arginyl hydrolases, since for all peptides examined the only cleavage site was the Arg-Xaa bond. We also demonstrated that Tc-OP and Tb-OP have a very specific carboxypeptidase activity for basic amino acids, which depends on the presence of at least of a pair of basic amino acids at the C-terminal end of the substrate. The peptide with triple Arg residues (Abz-AGRRRAQ-EDDnp) was an efficient substrate for Tc-OP and Tb-OP: the Arg-Ala peptide bond was cleaved first and then two C-terminal Arg residues were successively removed. The S1' subsite seems to be an important determinant of the specificity of both enzymes, showing a preference for Tyr, Ser, Thr and Gln as hydrogen donors. The presence of these amino acids at P1' resulted in substrates that were hydrolyzed with Km values in the sub-micromolar range. Taken together, this work supports the view that oligopeptidase B is a specialized protein-processing enzyme with a specific carboxypeptidase activity. Excellent substrates were obtained for Tb-OP and Tc-OP (Abz-AMRRTISQ-EDDnp and Abz-AHKRYSHQ-EDDnp resp.), which were hydrolyzed with remarkably high kcat and low Km values.
- IT 162851-86-7 198216-20-5 673501-88-7 673501-89-8 673501-95-6 673501-98-9

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(oligopeptidases B from Trypanosoma cruzi and Trypanosoma brucei are arginyl hydrolases)

RN 162851-86-7 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)-L-methionyl-L-isoleucyl-L-seryl-L-leucyl-L-methionyl-L-lysyl-L-arginyl-L-prolyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 198216-20-5 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)-L-leucylglycyl-L-methionyl-L-isoleucyl-L-seryl-L-leucyl-L-methionyl-L-lysyl-L-arginyl-L-prolyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RN 673501-88-7 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)-L-alanylglycylglycyl-L-arginylglycyl-L-alanyl-L-phenylalanyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

RN 673501-89-8 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)-L-alanylglycylglycyl-L-arginylglycyl-L-alanyl-L-tyrosyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 673501-95-6 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)-L-alanylglycylglycyl-L-arginylglycyl-L-alanyl-L-histidyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 673501-98-9 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)-L-alanylglycylglycyl-L-arginylglycyl-L-alanyl-L-prolyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

# RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 13 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 2003:405936 CAPLUS
- DN 139:246183
- TI Arylaminoethyl amides as inhibitors of the cysteine protease cathepsin K-investigating P'1 substituents
- AU Altmann, Eva; Green, Jonathan; Tintelnot-Blomley, Marina
- CS Arthritis & Bone Metabolism Therapeutic Area, Novartis Pharma AG, Basel, CH-4002, Switz.
- SO Bioorganic & Medicinal Chemistry Letters (2003), 13(12), 1997-2001 CODEN: BMCLE8; ISSN: 0960-894X
- PB Elsevier Science B.V.
- DT Journal
- LA English
- OS CASREACT 139:246183
- AB The synthesis and in vitro activities of a series of N $\alpha$ -benzyloxycarbonyl- and N $\alpha$ -acyl-L-leucine (2-phenylaminoethyl)amide derivs. which incorporate extended P1' substituents is described. Expanded lipophilic P1' moieties do not improve the potency of our inhibitors, however they generally lead to an increased specificity for cathepsin K over the two highly homologues cathepsins L and S. The appropriate combination of P3/P1t subunits results in highly potent cathepsin K inhibitors with an excellent selectivity profile.
- IT 289042-97-3P 289043-10-3P 289043-21-6P

289043-27-2P 289043-28-3P 289043-29-4P 289043-30-7P 289043-31-8P 289043-37-4P 289043-38-5P 289043-41-0P 289043-42-1P 289043-45-4P 289043-47-6P 289043-51-2P 289043-59-0P 289043-66-9P 289043-67-0P 596120-30-8P 596120-34-2P 596120-35-3P 596120-36-4P 596120-37-5P 596120-38-6P 596120-39-7P 596120-40-0P 596120-41-1P RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (preparation and mol. modeling of arylaminoethyl amides and their substituent effect on in-vitro activities as inhibitors of cysteine protease cathepsin K) 289042-97-3 CAPLUS RN CN Carbamic acid, [(1S)-3-methyl-1-[[[2-[[4-(phenylmethoxy)phenyl]amino]ethyl ]amino]carbonyl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 289043-10-3 CAPLUS

CN Carbamic acid, [(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 289043-21-6 CAPLUS

CN Carbamic acid, [(1S)-1-[[[2-[[4-(cyclopentyloxy)phenyl]amino]ethyl]amino]c arbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 289043-27-2 CAPLUS

CN Benzamide, 4-methoxy-N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 289043-28-3 CAPLUS

CN Benzamide, 4-ethyl-N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carb onyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 289043-29-4 CAPLUS

CN Benzamide, 4-ethyl-N-[(1S)-3-methyl-1-[[[2-[[4-(phenylmethoxy)phenyl]amino]ethyl]amino]carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 289043-31-8 CAPLUS
CN Carbamic acid, [(1S)-1-[[[2-[[4-[2-(1H-imidazol-1-yl)ethoxy]phenyl]amino]ethyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 289043-37-4 CAPLUS

CN Carbamic acid, [(1S)-3-methyl-1-[[[2-[[4-(2-methylpropoxy)phenyl]amino]eth yl]amino]carbonyl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 289043-38-5 CAPLUS

CN Carbamic acid, [(1S)-3-methyl-1-[[[2-[[4-(4-pyridinylmethoxy)phenyl]amino] ethyl]amino]carbonyl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 289043-41-0 CAPLUS

CN Carbamic acid, [(1S)-1-[[[2-[[4-(cyclopentylmethoxy)phenyl]amino]ethyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 289043-42-1 CAPLUS

CN Carbamic acid, [(1S)-1-[[[2-[[4-(cyclohexyloxy)phenyl]amino]ethyl]amino]ca rbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 289043-45-4 CAPLUS

CN Carbamic acid, [(1S)-1-[[[2-[[4-(cyclopropylmethoxy)phenyl]amino]ethyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 289043-47-6 CAPLUS

CN Carbamic acid, [(1S)-3-methyl-1-[[[2-[[4-[(tetrahydro-2H-pyran-4-yl)oxy]phenyl]amino]ethyl]amino]carbonyl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 289043-51-2 CAPLUS

CN Carbamic acid, [(1S)-3-methyl-1-[[[2-[[4-[(1-methyl-4-piperidinyl)oxy]phenyl]amino]ethyl]amino]carbonyl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 289043-59-0 CAPLUS

CN Carbamic acid, [(1S)-3-methyl-1-[[[2-[(4-phenoxyphenyl)amino]ethyl]amino]c arbonyl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 289043-66-9 CAPLUS

CN Benzamide, 4-methoxy-N-[(1S)-3-methyl-1-[[[2-[[4-(2-methylpropoxy)phenyl]amino]ethyl]amino]carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 289043-67-0 CAPLUS

CN Benzamide, N-[(1S)-1-[[[2-[[4-(cyclopentylmethoxy)phenyl]amino]ethyl]amino]carbonyl]-3-methylbutyl]-4-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 596120-30-8 CAPLUS

CN Carbamic acid, [(1S)-1-[[[2-[[4-[2-(dimethylamino)ethoxy]phenyl]amino]ethy l]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 596120-34-2 CAPLUS

CN Benzamide, N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 596120-35-3 CAPLUS

CN Benzamide, N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

RN 596120-36-4 CAPLUS

CN Benzamide, N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 596120-37-5 CAPLUS

CN Benzamide, 3-methoxy-N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 596120-38-6 CAPLUS

CN 1H-Indole-2-carboxamide, N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amin o]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 596120-39-7 CAPLUS

CN 1H-Indole-2-carboxamide, N-[(1S)-3-methyl-1-[[[2-[[4-(2-methylpropoxy)phenyl]amino]ethyl]amino]carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 596120-40-0 CAPLUS

CN 1H-Indole-2-carboxamide, N-[(1S)-1-[[[2-[[4-(cyclopentylmethoxy)phenyl]amino]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

RN 596120-41-1 CAPLUS

CN 1H-Indole-2-carboxamide, N-[(1S)-3-methyl-1-[[[2-[[4-(phenylmethoxy)phenyl]amino]ethyl]amino]carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

### RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 14 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 2003:325409 CAPLUS
- DN 139:285546
- TI Complementary use of ion trap/time-of-flight mass spectrometry in combination with capillary high-pressure liquid chromatography: Early characterization of in vivo metabolites of the cathepsin K inhibitor NVP-AAV490 in rat
- AU Blum, Wolfgang; Buhl, Thomas; Altmann, Eva; Kuhnol, Jurgen; Ramstein, Philippe; Aichholz, Reiner
- CS Research Department, Novartis Pharma AG, Basel, CH-4002, Switz.
- SO Journal of Chromatography, B: Analytical Technologies in the Biomedical and Life Sciences (2003), 787(2), 255-270
  CODEN: JCBAAI; ISSN: 1570-0232
- PB Elsevier Science B.V.
- DT Journal
- LA English
- AB Cathepsin K is a cysteine proteinase, primarily expressed in osteoclasts, which has a strong collagenolytic activity and plays an essential role involved in bone matrix degradation. Its inhibition could provide a novel approach to the treatment and prevention of osteoporosis. One structural class of lead compds. in our cathepsin K inhibitors program is based on an arylaminoethyl amide scaffold, which has potential metabolic weak points that might be stabilized by appropriate chemical modification(s). For the identification of potential metabolic "soft spots" and the rational design of improved derivs., early biotransformation of a potent arylaminoethyl amide cathepsin K inhibitor (NVP-AAV490-NX) was investigated in plasma, urine and liver homogenates of rats after i.v. bolus administration of 10 mg/kg. The detection and identification of metabolites was achieved by high-resolution mass spectrometry (time-of-flight MS) and multi-dimensional

mass spectrometry (ion trap MS). Both mass spectrometers were combined with reversed-phase capillary high-performance liquid chromatog. columns. It was demonstrated that both mass analyzers complement each other and that, even in the sub-nanogram range, the resulting set of MS data can be successfully used to elucidate most of the metabolic changes unambiguously, solely by mass spectrometric techniques. The proposed metabolite structures were addnl. corroborated by exact mass measurement of the protonated mol. ions to confirm the predicted elemental composition, by determination of the number of the exchangeable hydrogen atoms replacing water against deuterium oxide as mobile phase and, in one case, by an MS3 product ion experiment to elucidate the site of conjugation.

IT 609369-07-5 609369-09-7 609775-51-1 609775-53-3

RL: ANT (Analyte); ANST (Analytical study) (characterization of in vivo metabolites of the cathepsin K inhibitor NVP-AAV490 in rats)

RN 609369-07-5 CAPLUS

CN  $\beta$ -D-Glucopyranosiduronic acid, 4-[[2-[[(2S)-2-[[[1-(2-chlorophenyl)-1H-1,2,4-triazol-3-yl]carbonyl]amino]-4-methyl-1-oxopentyl]amino]ethyl]amino]phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

OH ر

....ОН

RN 609369-09-7 CAPLUS

CN 1H-1,2,4-Triazole-3-carboxamide, 1-(2-chlorophenyl)-N-[(1S)-1-[[[2-[(4-hydroxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

RN 609775-51-1 CAPLUS

CN 1H-1,2,4-Triazole-3-carboxamide, 1-(chlorohydroxyphenyl)-N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

D1-C1

D1-OH

RN 609775-53-3 CAPLUS

CN

β-D-Glucopyranosiduronic acid, 2(or 5)-methoxy-5(or`
2)-[[2-[[(2S)-4-methyl-1-oxo-2-[[(1-phenyl-1H-1,2,4-triazol-3-yl)carbonyl]amino]pentyl]amino]ethyl]amino]phenyl (9CI) (CA INDEX NAME)

IT 441052-62-6, NVP-AAV 490

RL: ANT (Analyte); PKT (Pharmacokinetics); ANST (Analytical study); BIOL (Biological study)

(characterization of in vivo metabolites of the cathepsin K inhibitor NVP-AAV490 in rats)

RN 441052-62-6 CAPLUS

CN 1H-1,2,4-Triazole-3-carboxamide, 1-(2-chlorophenyl)-N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

## RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:316623 CAPLUS

DN 139:303690

TI Specificity of S'1 and S'2 subsites of human tissue kallikrein using the reactive-centre loop of kallistatin: the importance of P'1 and P'2 positions in design of inhibitors

AU Pimenta, Daniel C.; Fogaca, Sandro E.; Melo, Robson L.; Juliano, Luiz; Juliano, Maria A.

CS Department of Biophysics, Escola Paulista de Medicina, Universidade Federal de Sao Paulo, Sao Paulo, 04044-020, Brazil

SO Biochemical Journal (2003), 371(3), 1021-1025 CODEN: BIJOAK; ISSN: 0264-6021

PB Portland Press Ltd.

DT Journal

LA English

We have demonstrated that the S'1 and S'2 subsites of human tissue AB kallikrein (hK1) play determinant roles in the recognition and hydrolysis of substrates. The presence of serine at position P'l and arginine at P'2 resulted in the best substrate, Abz-Ala-Ile-Lys-Phe-Phe-Ser-Arg-Gln-EDDnp, which was derived from the kallistatin reactive-center loop sequence and quencher groups o-aminobenzoic acid (Abz) and N-(2,4dinitrophenyl)ethylenediamine (EDDnp). Serine and arginine are also the residues at positions P'1 and P'2 in human kininogen, from which hK1 releases Lys-bradykinin. Several peptide analogs of Abz-Ala-Ile-Lys-Phe-Phe-Ser-Arg-Gln-EDDnp, in which the Ser and Arg residues were substituted with various other amino acids, were synthesized and tested as substrates. Most of them were hydrolyzed slowly, although they showed significant binding to hK1, as demonstrated by their competitive inhibition consts. (Ki). Using this information, six peptides were designed, synthesized and assayed as inhibitors of hK1. Abz-D-Lys-Phe-Phe-Pro-D-Arg-Gln-EDDnp, Abz-D-Lys-Phe-Arg-Pro-D-Arg-Gln-EDDnp and acetyl-D-Lys-Phe-Phe-Pro-Leu-Glu-NH2 inhibited hK1 in the range 20-30 nM. The peptide acetyl-D-Lys-Phe-Phe-Pro-Leu-Glu-NH2 was a weak inhibitor for other serine proteases, as indicated by the higher Ki values compared with hK1, but this peptide was a potent inhibitor of human plasma kallikrein, which has a Ki value of 8 This result was surprising, since this enzyme is known to be a restricted arginyl-hydrolase. In conclusion, acetyl-D-Lys-Phe-Pro-Leu-Glu-NH2 can be used as a leader compound to design specific inhibitors for hK1, plasma kallikrein, or for both at same time, if the inhibition of kinin release is the main goal.

IT 610767-59-4

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(anal. of human tissue kallikrein S'1 and S'2 subsite specificity using kallistatin-based peptide reveals importance of P'1 and P'2 positions in inhibitor design)

RN 610767-59-4 CAPLUS

CN  $L-\alpha$ -Glutamine, N-(2-aminobenzoyl)-L-alanyl-L-isoleucyl-L-lysyl-L-

phenylalanyl-L-phenylalanyl-L-seryl-L-prolyl-N-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:62809 CAPLUS

DN 138:250611

TI Nardilysin Cleaves Peptides at Monobasic Sites

AU Chow, K. Martin; Oakley, Oliver; Goodman, Jack; Ma, Zhangliang; Juliano, Maria Aparecida; Juliano, Luiz; Hersh, Louis B.

CS Department of Molecular and Cellular Biochemistry, University of Kentucky, Lexington, KY, USA

SO Biochemistry (2003), 42(7), 2239-2244 CODEN: BICHAW; ISSN: 0006-2960

PB American Chemical Society

DT Journal

LA English

AB Nardilysin (N-arginine dibasic convertase, EC 3.4.24.61) was first identified on the basis of its ability to cleave peptides containing an arginine dibasic pair, i.e., Arg-Arg or Arg-Lys. However, it was observed that an aromatic residue adjacent to the dibasic pair (i.e., Phe-Arg-Lys) could alter the cleavage site. In this study we determined whether nardilysin can cleave peptides at a single basic residue. Nardilysin cleaves β-endorphin at the monobasic site, Phel7-Lys18, with a kcat/Km of 2 + 108 M-1 min-1. This can be compared to a kcat/Km of 8.5 + 108 M-1 min-1 for cleavage between a dibasic pair in dynorphin B-13. Nardilysin also cleaves calcitonin at His-Arg and somatostatin-14 at Cys-Lys. We examined the hydrolysis of fluorogenic peptides based on the β-endorphin 12-24 sequence, Abz-T-P-L-V-T-L-X1-X2-N-A-I-I-K-Q-EDDnp. Nardilysin hydrolyzes the peptides when X1-X2 = F-K, F-R, W-K, M-K, Y-K,

and L-K. The kinetics of cleavage at F-K and F-R are similar; however, K-F is not hydrolyzed. Nardilysin cleaves at two monobasic sites M-K and F-R of the kallidin model peptide Abz-MISLMKRPPGFSPFRSSRI-NH2, releasing desArg10 kallidin (KRPPGFSPF). However, nardilysin does not release desArg10 kallidin from the physiol. precursor low mol. weight kininogen. These studies extend the range of potential substrates for nardilysin and further substantiate that nardilysin is a true peptidase.

IT 162851-86-7

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(nardilysin cleaves peptides at monobasic sites)

RN 162851-86-7 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)-L-methionyl-L-isoleucyl-L-seryl-L-leucyl-L-methionyl-L-lysyl-L-arginyl-L-prolyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

PAGE 1-A

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:795658 CAPLUS

DN 138:280690

- TI Interaction of heparin with internally quenched fluorogenic peptides derived from heparin-binding consensus sequences, kallistatin and anti-thrombin III
- AU Pimenta, Daniel C.; Nantes, Iseli L.; De Souza, Eduardo S.; Le Bonniec, Bernard; Ito, Amando S.; Tersariol, Ivarne L. S.; Oliveira, Vitor; Juliano, Maria A.; Juliano, Luiz
- CS Centro de Toxicologia Aplicada, CAT/CEPID, Sao Paulo, 05503-900, Brazil

SO Biochemical Journal (2002), 366(2), 435-446

CODEN: BIJOAK: ISSN: 0264-6021

- PB Portland Press Ltd.
- DT Journal
- LA English
- Internally quenched fluorogenic (IQF) peptides bearing the fluorescence AB donor/acceptor pair o-aminobenzoic acid (Abz)/N-(2,4dinitrophenyl)ethylenediamine (EDDnp) at N- and C-terminal ends were synthesized containing heparin-binding sites from the human serpins kallistatin and antithrombin, as well as consensus heparin-binding sequences (Cardin clusters). The dissociation constant (Kd), as well as the stoichiometry for the heparin-peptide complexes, was determined directly by measuring the decrease in fluorescence of the peptide solution Exptl. procedures were as sensitive as those used to follow the fluorescence change of tryptophan in heparin-binding proteins. The conformation of the peptides and the heparin-peptide complexes were obtained from measurements of time-resolved fluorescence decay and CD spectra. Kallistatin (Arg300-Pro319)-derived peptide (HC2) and one derived from antithrombin III helix D [(AT3D), corresponding to Ser112-Lys139], which are the heparin-binding sites in these serpins, showed significant affinity for 4500 Da heparin, for which Kd values were 17 nM and 100 nM, resp. The CD spectra of the heparin-HC2 peptide complex did not show any significant α-helix content, different from the situation with peptide AT3D, for which complex-formation with heparin resulted in 24% α-helix content. The end-to-end distance distribution and the time-resolved fluorescence-decay measurements agree with the CD spectra and Kd values. The synthetic  $\alpha$ -Me glycoside pentasaccharide AGA\*IAM (where A represents N,6-O-sulfated  $\alpha$ -D-glucosamine; G,  $\beta$ -D-glucuronic acid; A\*, N,3,6-O-sulfated  $\alpha$ -D-glucosamine; I, 2-O-sulfated  $\alpha\text{-L-iduronic}$  acid; and AM,  $\alpha\text{-Me}$  glycoside of A) also binds to AT3D and other consensus heparin-binding sequences, although with lower The interaction of IQF peptides with 4500 Da heparin was affinity. displaced by protamine. In conclusion, IQF peptides containing Abz/EDDnp as the donor/acceptor fluorescence pair are very promising tools for structure-activity relationship studies on heparin-peptide complexes, as well as for the development of new peptides as heparin reversal-effect compds.

#### IT 503816-84-0 503816-85-1

RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(interaction of heparin with internally quenched fluorogenic peptides derived from heparin-binding consensus sequences, kallistatin and anti-thrombin III)

RN 503816-84-0 CAPLUS

CN L-Glutamamide, N2-(2-aminobenzoyl)-L-arginyl-L-tryptophyl-L-asparaginyl-L-asparaginyl-L-asparaginyl-L-leucyl-L-leucyl-L-arginyl-L-arginyl-L-asparaginyl-L-phenylalanyl-L-tyrosyl-L-lysyl-L-leucyl-L-α-glutamyl-L-leucyl-L-histidyl-L-leucyl-L-prolyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]-(9CI) (CA INDEX NAME)

PAGE 1-D

RN 503816-85-1 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)-L-phenylalanyl-L-asparaginyl-L-leucyl-L-threonyl-L- $\alpha$ -glutamyl-L-leucyl-L-seryl-L- $\alpha$ -glutamyl-L-seryl-L- $\alpha$ -aspartyl-L-valyl-L-histidyl-L-arginylglycyl-L-phenylalanyl-L-glutaminyl-L-histidyl-L-leucyl-L-leucyl-L-histidyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-D

# RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 18 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 2002:783113 CAPLUS
- DN 138:182961
- TI Discriminating between the Activities of Human Neutrophil Elastase and Proteinase 3 Using Serpin-derived Fluorogenic Substrates
- AU Korkmaz, Brice; Attucci, Sylvie; Hazouard, Eric; Ferrandiere, Martine; Jourdan, Marie Lise; Brillard-Bourdet, Michele; Juliano, Luiz; Gauthier, Francis
- CS INSERM EMI-U 0010, Proteases et Vectorisation, Univ. François Rabelais, Tours, 37032, Fr.

SO Journal of Biological Chemistry (2002), 277(42), 39074-39081 CODEN: JBCHA3; ISSN: 0021-9258

PB American Society for Biochemistry and Molecular Biology

DT Journal

LA English

AB Human neutrophil elastase (HNE) has long been linked to the pathol. of a variety of inflammatory diseases and therefore is a potential target for therapeutic intervention. At least two other serine proteases, proteinase 3 (Pr3) and cathepsin G, are stored within the same neutrophil primary granules as HNE and are released from the cell at the same time at inflammatory sites. HNE and Pr3 are structurally and functionally very similar, and no substrate is currently available that is preferentially cleaved by Pr3 rather than HNE. Discrimination between these two proteases is the first step in elucidating their relative contributions to the development and spread of inflammatory diseases. Therefore, we have prepared new fluorescent peptidyl substrates derived from natural target proteins of the serpin family. This was done because serpins are rapidly cleaved within their reactive site loop whether they act as protease substrates or inhibitors. The hydrolysis of peptide substrates reflects the specificity of the parent serpin including those from α-1-protease inhibitor and monocyte neutrophil elastase inhibitor, two potent inhibitors of elastase and Pr3. More specific substrates for these proteases were derived from the reactive site loop of plasminogen activator inhibitor 1, proteinase inhibitors 6 and 9, and from the related viral cytokine response modifier A (CrmA). This improved specificity was obtained by using a cysteinyl residue at P1 for Pr3 and an Ile residue for HNE and because of occupation of protease S' subsites. These substrates enabled us to quantify nanomolar concns. of HNE and Pr3 that were free in solution or bound at the neutrophil surface. As membrane-bound proteases resist inhibition by endogenous inhibitors, measuring their activity at the surface of neutrophils may be a great help in understanding their role during inflammation.

#### IT 497952-75-7 497952-77-9

RL: BSU (Biological study, unclassified); BIOL (Biological study) (serpin-derived fluorogenic substrates permit discrimination between activities of human neutrophil elastase and proteinase 3)

RN 497952-75-7 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)-L-α-glutamyl-L-alanyl-L-isoleucyl-L-prolyl-L-methionyl-L-seryl-L-isoleucyl-L-prolyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

RN 497952-77-9 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)-L- $\alpha$ -glutamyl-L-alanyl-L-isoleucyl-L-prolyl-(2S)-2-amino-4-(methylsulfinyl)butanoyl-L-seryl-L-isoleucyl-L-prolyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RE.CNT 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN

- AN 2002:723192 CAPLUS
- DN 138:102752
- TI Temperature and salts effects on the peptidase activities of the recombinant metallooligopeptidases neurolysin and thimet oligopeptidase
- AÚ Oliveira, Vitor; Gatti, Reynaldo; Rioli, Venessa; Ferro, Emer S.; Spisni, Alberto; Camargo, Antonio C. M.; Juliano, Maria A.; Juliano, Luiz
- CS Department of Biophysics, Escola Paulista de Medicina, Sao Paulo, Brazil
- SO European Journal of Biochemistry (2002), 269(17), 4326-4334 CODEN: EJBCAI; ISSN: 0014-2956
- PB Blackwell Science Ltd.
- DT Journal
- LA English
- AB We report the recombinant neurolysin and thimet oligopeptidase (TOP) hydrolytic activities towards internally quenched fluorescent peptides derived from the peptide Abz-GGFLRRXQ-EDDnp (Abz, ortho-aminobenzoicacid; EDDnp, N-(2,4-dinitrophenyl) ethylenediamine), in which X was substituted by 11 different natural amino acids. Neurolysin hydrolyzed these peptides at R-R or at R-X bonds, and TOP hydrolyzed at R-R or L-R bonds, showing a preference to cleave at three or four amino acids from the C-terminal end. The kinetic parameters of hydrolysis and the variations of the cleavage sites were evaluated under different conditions of temperature and salt concentration

The relative amount of cleavage varied with the nature of the substitution at the X position as well as with temperature and NaCl concentration TOP was activated

by all assayed salts in the range 0.05-0.2 M for NaCl, KCl, NH4Cl and NaI, and 0.025-0.1 M for Na2SO4. Concentration higher than 0.2 N NH4Cl and NaI reduced TOP activity, while 0.5 N or higher concentration of NaCl, KCl and Na2SO4

increased TOP activity. Neurolysin was strongly activated by NaCl, KCl and Na2SO4, while NH4Cl and NaI have very modest effect. High pos. values of enthalpy ( $\Delta H^*$ ) and entropy ( $\Delta S^*$ ) of activation were found together with an unusual temperature dependence upon the hydrolysis of the substrates. The effects of low temperature and high NaCl concentration on the hydrolytic activities of neurolysin and TOP do not seem to be a consequence of large secondary structure variation of the proteins, as indicated by the far-UV CD spectra. However, the modulation of the activities of the two oligopeptidases could be related to variations of conformation, in limited regions of the peptidases, enough to modify their activities.

### IT 486406-43-3 486406-44-4 486406-45-5 486406-46-6

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(kinetic parameters of hydrolysis and variations of cleavage sites of series of internally quenched fluorescent peptides by recombinant metallooligopeptidases neurolysin and thimet oligopeptidase in different conditions of temperature and salts)

RN 486406-43-3 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)glycylglycyl-L-phenylalanyl-L-leucyl-L-arginyl-L-arginyl-L-histidyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 486406-44-4 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)glycylglycyl-L-phenylalanyl-L-leucyl-L-arginyl-L-arginyl-L-tyrosyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H & NH_2 \\ \hline O & NH & H \\ \hline S & N & S & H \\ \hline & i-Bu & O \\ \end{array}$$

RN 486406-45-5 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)glycylglycyl-L-phenylalanyl-L-leucyl-L-arginyl-L-phenylalanyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

### PAGE 1-A

RN 486406-46-6 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)glycylglycyl-L-phenylalanyl-L-leucyl-L-arginyl-L-prolyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

$$\begin{array}{c|c} & H & NH_2 \\ \hline S & O & NH & NH_2 \\ \hline S & NH & O_2N & NO_2 \\ \hline N & NH & NH_2 & NO_2 \\ \hline N & NH & NH_2 & NO_2 \\ \hline N & NH & NH_2 & NO_2 \\ \hline N & NH & NH_2 & NO_2 \\ \hline N & NH & NH_2 & NO_2 \\ \hline N & NH & NH_2 & NO_2 \\ \hline N & NH & NH_2 & NO_2 \\ \hline N & NH & NH_2 & NH_2 \\ \hline N & NH_2 & NH_2 \\ \hline N & NH_2 & NH_2 \\ \hline N & NH_$$

RE.CNT 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 20 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 2002:348238 CAPLUS
- DN 137:79205
- TI Arylaminoethyl Amides as Novel Non-Covalent Cathepsin K Inhibitors
- AU Altmann, Eva; Renaud, Johanne; Green, Jonathan; Farley, David; Cutting, Brian; Jahnke, Wolfgang

CS Arthrithis & Bone Metabolism Therapeutic Area and Central Technologies, Novartis Pharma Research, Basel, CH-4002, Switz.

SO Journal of Medicinal Chemistry (2002), 45(12), 2352-2354 CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

OS CASREACT 137:79205

AB A series of Nα-benzyloxycarbonyl- and Nα-acyl-L-leucine
(2-arylaminoethyl)amides, I (R = H, 3-Me, 4-Me, 3-Cl, 4-Cl, 3-OMe, 4-OMe)
and II [R1 = 4-MeOC6H4, 4-PhCH2OC6H4, 4-PrC6H4, 4-(isoPr)C6H4,
5-isopropyl-2-pyridinyl, 4-(1-hydroxyethyl)phenyl, 1-(2-chlorophenyl)1,2,4-triazol-3-yl, 1-(2,3-dichlorophenyl)-1,2,4-triazol-3-yl], were
prepared and evaluated for their inhibitory activity against rabbit and
human cysteine proteases cathepsins K, L, and S. The data obtained by the
authors indicate that II represents a new class of selective non-covalent
inhibitors of cathepsin K. For example, II [R1 = 4-PhCH2OC6H4,
5-isopropyl-2-pyridinyl, 1-(2-chlorophenyl)-1,2,4-triazol-3-yl]
demonstrated high potency toward rabbit and human cathepsin K (IC50 <
0.006 μM) and were characterized by an excellent selectivity profile
vs. human cathepsins L and S.

IT 289043-10-3P

RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation and biol. activity of N-acylleucine (arylaminoethyl) amides as non-covalent inhibitors of cathepsin K, L and S)

RN 289043-10-3 CAPLUS

CN Carbamic acid, [(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 289043-05-6P 289043-06-7P 289043-07-8P 289043-09-0P 289043-11-4P 289043-13-6P 289043-27-2P 289044-17-3P 289044-26-4P 441052-60-4P 441052-61-5P 441052-62-6P 441052-63-7P 441052-68-2P 441052-83-1P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and biol. activity of N-acylleucine (arylaminoethyl)amides as non-covalent inhibitors of cathepsin K, L and S)

RN 289043-05-6 CAPLUS

CN Carbamic acid, [(1S)-1-[[[2-[(4-chlorophenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 289043-06-7 CAPLUS

CN Carbamic acid, [(1S)-3-methyl-1-[[[2-[(3-methylphenyl)amino]ethyl]amino]ca rbonyl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 289043-07-8 CAPLUS

CN Carbamic acid, [(1S)-3-methyl-1-[[[2-[(4-methylphenyl)amino]ethyl]amino]carbonyl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN 289043-09-0 CAPLUS

CN Carbamic acid, [(1S)-1-[[[2-[(3-chlorophenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 289043-11-4 CAPLUS

CN Carbamic acid, [(1S)-1-[[[2-[(3-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 289043-13-6 CAPLUS

CN Carbamic acid, [(1S)-3-methyl-1-[[[2-(phenylamino)ethyl]amino]carbonyl]but yl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 289043-27-2 CAPLUS

CN Benzamide, 4-methoxy-N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 289044-17-3 CAPLUS

CN Benzamide, N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]-4-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 289044-26-4 CAPLUS

CN Benzamide, N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 441052-60-4 CAPLUS

CN 2-Pyridinecarboxamide, N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]-5-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 441052-61-5 CAPLUS

CN Benzamide, 4-(1-hydroxyethyl)-N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

RN 441052-62-6 CAPLUS

CN 1H-1,2,4-Triazole-3-carboxamide, 1-(2-chlorophenyl)-N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 441052-63-7 CAPLUS

CN 1H-1,2,4-Triazole-3-carboxamide, 1-(2,3-dichlorophenyl)-N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 441052-68-2 CAPLUS

CN 1H-1,2,4-Triazole-3-carboxamide, 1-(2-chlorophenyl)-N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl-13C]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 441052-83-1 CAPLUS

CN Benzamide, N-[(1S)-1-[[[2-[(4-methoxyphenyl)amino]ethyl]amino]carbonyl]-3-methylbutyl]-4-propyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 441052-58-0 CMF C25 H35 N3 O3

$$\begin{array}{c|c} & & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

#### THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 14 ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 21 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN L4

AN 2002:122964 CAPLUS

DN 136:167384

ΤI Preparation of 4-pyrimidinamines as neuroprotectants.

Grant, Elfrida R.; Brown, Frank K.; Zivin, Robert Allan; McMillan, IN Michael; Zhong, Zhong; Scott, Malcolm; Reitz, Allen B.; Ross, Tina Morgan

PA Ortho-McNeil Pharmaceutical, Inc., USA

SO PCT Int. Appl., 92 pp.

CODEN: PIXXD2

 $\mathsf{DT}$ Patent

LΑ English

	FAN.	CNT	1																	
PATENT NO.				KIN	D	DATE			APPL	ICAT	ION	NO.		D	ATE					
	PI WO 2002012198 WO 2002012198			A2 20020214		WO 2001-US24659					20010806									
				A3 20020606																
			W:	AE,	AG,	AL,	AM,	ΑT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN.	
				co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
				GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	
				LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT,	
				RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	UZ,	
				VN,	YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM				
			RW:	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	ΑT,	BE,	CH,	CY,	
				DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,	
				ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG		
							US 2000-223791P			P 20000808										
	CA 2419030		AA 20020214			CA 2001-2419030					20010806									
						US 2000-223791P				I	P 20000808									
							1	WO 2	001-1	US24	659	V	N 20	00108	806					
AU 2001081120		A5 20020218		AU 2001-81120					20010806											
						US 2000-223791P				I	P 20000808									
											1	WO 2	001-1	US24	659	V	W 20	0010	806	
		US	2003	0088	83		A1		2003	0109	1	US 2	001-	9228	74		20	00108	806	

EP 1313713	A2	20030528	US 2000-223791P EP 2001-959581	P	20000808 20010806
R: AT, BE, CH,	DE,		GB, GR, IT, LI, LU, NL	, S	E, MC, PT,
,,		,	US 2000-223791P	P	20000808
			WO 2001-US24659	W	20010806
BR 2001013165	Α	20030715	BR 2001-13165		20010806
			US 2000-223791P	P	20000808
			WO 2001-US24659 ·	W	20010806
JP 2004505952	T2	20040226	JP 2002-518176		20010806
			US 2000-223791P	P	20000808
			WO 2001-US24659	W	20010806
NZ 524100	Α	20050128	NZ 2001-524100	_	20010806
			US 2000-223791P	P	20000808
			WO 2001-US24659	W	20010806
ZA 2003001868	Α	20040625	ZA 2003-1868	_	20030306
			US 2000-223791P	P	20000808
US 2003212079	A1	20031113	US 2003-396158		20030325
			US 2000-223791P	P	20000808
•			US 2001-922874	A3	20010806
US 2004006094	A1	20040108	US 2003-395971	_	20030325
			US 2000-223791P	P	
			US 2001-922874	Α3	20010806

OS MARPAT 136:167384

AB Pharmaceutical compns. comprising a pharmaceutically acceptable carrier [I; R9 = H, thienyl, furanyl, pyrrolyl, (substituted) Ph, pyridinyl,
pyridinyl, naphthyl, benzo[b]thien-2-yl, 2-benzofuranyl, pyrimidinyl, 2,4-bis(methoxyphenyl)-5-pyrimidinyl; R10 = cyanoalkyl, alkylamino, dialkylamino, hydroxyalkylamino, hydroxydialkylamino; R11 = H, alkyl], are claimed. Thus, a mixture of N-(2-aminoethyl)-N'-(6-biphenyl-3-ylpyrimidin-4yl)-N-ethylbenzene-1,4-diamine (preparation given), N-benzoylalanine, diisopropylethylamine, HBTU, and DMF was stirred overnight at room temperature to give N-[1-[[2-[4-(6-biphenyl-3-ylpyrimidin-4ylamino) phenyl] ethylamino] ethylcarbamoyl] ethyl] benzamide. Tested compds. in a differentiated P19 cell assay using 3 mM glutamate showed neuroprotectant activity with IC50 = 0.07  $\mu$ M to >1  $\mu$ M. IT

397850-34-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 4-pyrimidinamines as neuroprotectants)

RN 397850-34-9 CAPLUS

CNBenzamide, N-[2-[[2-[[4-[(6-[1,1'-biphenyl]-3-yl-4pyrimidinyl)amino]phenyl]ethylamino]ethyl]amino]-1-methyl-2-oxoethyl]-(9CI) (CA INDEX NAME)

L4ANSWER 22 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN AN 2001:937212 CAPLUS

DN 136:345906

Enantiomerization of 3-carbethoxy-1,4-benzodiazepin-2-one: combined chiral TI HPLC and spectroscopic study

Abatangelo, Anna; Zanetti, Flavio; Navarini, Luciano; Kontrec, Darko; AU Vinkovic, Vladimir; Sunjic, Vitomir POLYtech, Trieste, Italy

CS

Chirality (2002), 14(1), 12-17 SO CODEN: CHRLEP; ISSN: 0899-0042

PB Wiley-Liss, Inc.

Journal DT

English LΑ

Recently developed chiral HPLC columns CHIRIS AD1 and CHIRIS AD2 have been AB demonstrated to sep. racemic, configurationally unstable ethyl-7-chloro-2-oxo-5-phenyl-2,3-dihydro-1H-1,4-benzodiazepine-3carboxylate (1) and its 3-Me congener 2; fast on-column enantiomerization of configurationally unstable 1 was observed, however. Addition of 0.1% of

AcOH

to the eluting mixture inhibits enantiomerization, whereas the same percentage of Et3N completely precludes enantiosepn., suggesting base-catalysis by free β-aminoethyl groups, present in low percentage in chiral stationary phase (CSP). When both CSPs were prepared under conditions of nonexhaustive acylation by N-DNB- $\alpha$ -amino acids, no separation of 1 was observed The rate of enantiomerization of CHIRIS AD2 was determined at 25°C, the mechanism is discussed, and exptl. results correlated with calculated relative stabilities of the tautomers la-c.

Absolute

(3S) configuration of (+) enantiomers of 1 and 2 was determined by comparison of their elution profile to that of  $(\pm)$ -3 and (3S)-(+)-3, taking into account relative (wa or we) configuration of the prevailing conformer in solution

416898-21-0D, reaction products with silica 416898-22-1D ΙT , reaction products with silica

RL: ARU (Analytical role, unclassified); ANST (Analytical study) (resolution of 1.4-benzodiazepine derivs. by HPLC and spectroscopy using DNB- $\alpha$ -amino acid as chiral selectors)

RN 416898-21-0 CAPLUS

Benzeneacetamide, N-[2-[[3-amino-5-[(2-aminoethyl)amino]-2,4,6-CN tricyanophenyl]amino]ethyl]- $\alpha$ -[(3,5-dinitrobenzoyl)amino]-,  $(\alpha R)$  - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$H_2N$$
 $H_2N$ 
 $H_2N$ 
 $H_2N$ 
 $H_3N$ 
 $H_2N$ 
 $H_3N$ 
 $H_3N$ 

RN 416898-22-1 CAPLUS

Benzamide, N-[(1R)-1-[[[2-[[3-amino-5-[(2-aminoethyl)amino]-2,4,6-CN tricyanophenyl]amino]ethyl]amino]carbonyl]-3-methylbutyl]-3,5-dinitro-

#### (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$H_2N$$
 $H_2N$ 
 $H_2N$ 

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 23 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:895668 CAPLUS

DN 136:19946

TI Amidomalonamides useful as inhibitors of matrix metalloproteinase (MMPs)

IN Warshawsky, Alan M.; Janusz, Michael J.

PA Aventis Pharmaceuticals Inc., USA

SO U.S., 28 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
					-		
ΡI	US 6329550	B1	20011211	US 1999-464907		19991217	
				US 1998-172246P	P	19981231	

OS MARPAT 136:19946

The present invention provides the title compds. [I; R1, R2 = independently H, C1-C10 alkyl, (CH2)a-Ar1, (CH2)b-Ar2 (wherein a = 1-6; b = 2-6; Ar1 = (un)substituted Ph, naphthyl, pyridyl; Ar2 = (un)substituted anilino); R3 = C1-C6 alkyl, (CH2)mW, (CH2)pAr3, etc. (wherein m = 2-8; p = 0-10; W = phthalimido; Ar3 = (un)substituted Ph, thienyl, pyridyl, etc.); R4 = H, C(O)R10, C(O)(CH2)qK, SG (wherein R10 = H, C1-C4 alkyl, Ph, CH2Ph; q = 0-2; K = pyridyl, imidazolyl, etc.; G = 2-pyridyl, (CH2)wpyridyl, etc. (wherein w = 1-3))], stereoisomers, and pharmaceutically acceptable salts and hydrates thereof which are useful for inhibiting matrix metalloproteinases (no data). Thus, amidomalonamide II was prepared over 5 steps from t-butoxycarbonylaminomalonic acid. Compds. I are effective at 1-100 mg/kg/day.

IT 378789-30-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of amidomalonamides useful as inhibitors of matrix metalloproteinase (MMPs))

RN 378789-30-1 CAPLUS

CN Propanediamide, 2-[[(2S)-2-mercapto-1-oxo-3-phenylpropyl]amino]-N,N'-bis[2-(phenylamino)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 283149-70-2P 378789-29-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of amidomalonamides useful as inhibitors of matrix metalloproteinase (MMPs))

RN 283149-70-2 CAPLUS

CN Propanediamide, 2-[[(2R)-2-bromo-1-oxo-3-phenylpropyl]amino]-N,N'-bis[2-(phenylamino)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 378789-29-8 CAPLUS

CN Ethanethioic acid, S-[(1S)-2-oxo-2-[[2-oxo-2-[[2-(phenylamino)ethyl]amino]-1-[[[2-(phenylamino)ethyl]amino]carbonyl]ethyl]amino]-1-(phenylmethyl)ethyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 24 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:677356 CAPLUS

DN 135:195790

TI Preparation of peptides which inhibit human tissue kallikrein and the liberation of kinins

IN De Nucci, Gilberto; Juliano Neto, Luiz; Giuseppe, Caliendo; Vincenzo, Santagada

PA Laboratorios Biosintetica Ltda, Brazil; Universidade Federal de Sao Paulo
-UNIFESP

SO Braz. Pedido PI, 11 pp.

CODEN: BPXXDX

DT Patent

LA Portuguese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	BR 9900694	Α	20001017	BR 1999-694	19990308		
				BR 1999-694	19990308		

AB Analogs of o-H2NC6H4CO-Phe-Arg-Arg-Pro-NHCH2CH2NHC6H3(NO2)2-2,4 and peptides PhCH2CO-X-Ser-Arg-NH2 (X represents certain non-natural amino acids) were prepared as inhibitors of human tissue kallikrein and the liberation of kinins for use as inflammation inhibitors and analgesics. Thirty claimed compds. were prepared by the solid-phase method.

IT 189621-46-3P 189621-51-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of peptides which inhibit human tissue kallikrein and the liberation of kinins)

RN 189621-46-3 CAPLUS

CN L-Argininamide, N-(2-aminobenzoyl)-L-phenylalanyl-L-arginyl-L-prolyl-N-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 189621-51-0 CAPLUS

CN L-Argininamide, N-(2-aminobenzoyl)-L-phenylalanyl-L-arginyl-L-prolyl-N-(2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

- L4 ANSWER 25 OF 83 CAPLUS , COPYRIGHT 2005 ACS on STN
- AN 2001:519039 CAPLUS
- DN 135:284863
- TI Substrate specificity of recombinant cysteine proteinase, CPB, of Leishmania mexicana
- AU Alves, L. C.; Judice, W. A. S.; St. Hilaire, P. M.; Meldal, M.; Sanderson, S. J.; Mottram, J. C.; Coombs, G. H.; Juliano, L.; Juliano, M. A.
- CS Department of Biophysics, Escola Paulista de Medicina, Universidade Federal de Sao Paulo, Sao Paulo, 04044-020, Brazil
- SO Molecular and Biochemical Parasitology (2001), 116(1), 1-9 CODEN: MBIPDP; ISSN: 0166-6851

PB Elsevier Science Ireland Ltd.

DT Journal

LA English

The primary S1 subsite specificity of a recombinant cysteine proteinase, AB CPB2.8ACTE, of Leishmania mexicana was investigated in a systematic way using a series of peptides derived from Abz-KLRFSKQ-EDDnp in which Arg was substituted by all natural amino acids (where Abz is ortho-amino-benzoyl and EDDnp is N-[2,4-dinitrophenyl]-ethylenediamine). The peptides from this series with charged side chain amino acids, Cys, Cys(SBzl), and Thr(OBzl) were well hydrolyzed. All other substitutions resulted in peptides that were resistant or hydrolyzed very slowly and inhibited the enzyme with Ki values in the range of 9-400 nM. Looking for natural substrates for CPB2.8, we observed that the recombinant enzyme failed to release kinin from human kininogen, an activity earlier observed with cruzipain from Trypanosoma cruzi (Del Nery et al., J. Biol. Chemical 272 (1997) 25713.). This lack of activity seems to be a result of the resistance to hydrolysis of the sequence at the N-terminal site of bradykinin in the human kininogen. The preferences for the S3, S2 and S1'-S3' for some amino acids were also examined using substrates derived from Abz-KLRFSKQ-EDDnp with variations at Lys, Leu, Phe, Ser and Lys, using the amino acids Ala, Phe, Leu, His or Pro. Peptides with Phe at Pl' presented the highest affinity to the leishmanial enzyme. For comparison, some of the obtained peptides were also assayed with recombinant human cathepsin L and cruzain. The best substrates for CPB2.8ACTE were also well hydrolyzed by cathepsin L, however, the best inhibitors of the parasite enzyme have low affinity to cathepsin L. These promising data provide leads for the design of anti-parasitic drugs directed against the leishmanial enzyme.

#### IT 364630-61-5

CN

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study) (substrate specificity of cysteine proteinase CPB from Leishmania mexicana provides leads for design of anti-parasitic drugs)

RN 364630-61-5 CAPLUS

L-Glutamamide, N2-(2-aminobenzoyl)-L-lysyl-L-leucyl-L-arginyl-L-phenylalanyl-L-seryl-L-phenylalanyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]-(9CI) (CA INDEX NAME)

### IT 162851-86-7 364630-60-4

RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)

(substrate specificity of cysteine proteinase CPB from Leishmania mexicana provides leads for design of anti-parasitic drugs)

RN 162851-86-7 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)-L-methionyl-L-isoleucyl-L-seryl-L-leucyl-L-methionyl-L-lysyl-L-arginyl-L-prolyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RN 364630-60-4 CAPLUS

CN L-Glutamamide, N2-(2-aminobenzoyl)-L-lysyl-L-leucyl-L-arginyl-L-phenylalanyl-L-seryl-L-prolyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]-(9CI) (CA INDEX NAME)

$$H_{2N}$$
 $H_{2N}$ 
 $H$ 

PAGE 1-B

# RE.CNT 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 26 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:402359 CAPLUS

DN 135:174386

TI Solid-phase synthesis of chiral stationary phases based on 2,4,5,6-tetrachloro-1,3-dicyanobenzene derivatives spaced from N-3,5-dinitrobenzoyl  $\alpha$ -amino acids: comparative study of their resolution efficacy

AU Kontrec, Darko; Abatangelo, Anna; Vinkovic, Vladimir; Sunjic, Vitomir

CS Ruder Boskovic Institute, Zagreb, HR-10002, Croatia

SO Chirality (2001), 13(6), 294-301 CODEN: CHRLEP; ISSN: 0899-0042

PB Wiley-Liss, Inc.

DT Journal

LA English

AB Two new chiral stationary phases, 3-[5-chloro-1,3-dicyano-2,4-[2'-(N'-1,3-dinitrobenzoyl-D-phenylglycinyl) aminoethyl]aminophen-1-yl] aminopropyl silica (CSP-1) and 3-[5-chloro-1,3-dicyano-2,4-[2'-(N'-1,3-dinitrobenzoyl-L-leucinyl)aminoethyl] aminophen-1-yl] aminopropyl silica (CSP-2), were prepared by solid-phase synthesis. They comprise chiral unit, 3,5-dinitrobenzoyl derivative of the amino acid, D-PhGly or L-Leu, bound via

spacer 1,2-diaminoethane to 2,4-positions of the persubstituted benzene ring, derived from compound 1, and possess pseudo-C2 symmetry. Preparation of model compds. 6 and 7 confirmed the structure of chiral selectors, which comprise  $\pi$ -donor persubstituted aromatic ring and two strong  $\pi$ -acceptor 3,5-dinitrobenzoyl amido units. CD spectra of model selectors 6 and 7, run in DMSO >250 nm, exhibit neg. exciton coupling (EC) between  $\pi$ -acceptor and  $\pi$ -donor chromophores, C1 sym. model compound 8 exhibited much weaker EC and 9, devoid of  $\pi$ -donor unit, does not exhibit any significant CD. Combined  $\pi$ -donor and  $\pi$ -acceptor properties enable the new CSPs to sep. a broad range of racemates. The columns with CSP-1 and CSP-2 were tested for the separation of 22 racemates by HPLC with two different mobile phase systems and the results are compared with those obtained by using a structurally related com. column.

IT 353524-61-5P 353524-62-6P 353524-63-7P 353524-65-9P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in preparation of model compds. for chiral stationary phases based on 2,4,5,6-tetrachloro-1,3-dicyanobenzene derivs. spaced from N-3,5-dinitrobenzoyl  $\alpha$ -amino acids)

RN 353524-61-5 CAPLUS

CN Benzeneacetamide, N,N'-[(5-butyl-4-chloro-2,6-dicyano-1,3-phenylene)bis(imino-2,1-ethanediyl)]bis[ $\alpha$ -[(3,5-dinitrobenzoyl)amino]-, ( $\alpha$ R, $\alpha$ 'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

RN 353524-62-6 CAPLUS

CN Benzeneacetamide, N,N'-[(4-chloro-2,6-dicyano-5-dodecyl-1,3-phenylene)bis(imino-2,1-ethanediyl)]bis[ $\alpha$ -[(3,5-dinitrobenzoyl)amino]-, ( $\alpha$ R, $\alpha$ 'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

$$O_2N$$
 $H$ 
 $N$ 
 $R$ 
 $H$ 
 $N$ 
 $N$ 
 $H$ 
 $N$ 
 $N$ 
 $H$ 
 $N$ 
 $N$ 
 $H$ 
 $N$ 
 $H$ 
 $N$ 
 $N$ 
 $H$ 
 $N$ 
 $N$ 
 $H$ 
 $N$ 
 $N$ 
 $H$ 
 $N$ 
 $H$ 
 $N$ 
 $N$ 
 $H$ 
 $N$ 

PAGE 1-B

RN 353524-63-7 CAPLUS

CN Benzeneacetamide,  $\alpha$ -[(3,5-dinitrobenzoyl)amino]-N-[2-[(2,3,5-trichloro-4,6-dicyanophenyl)amino]ethyl]-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 353524-65-9 CAPLUS

CN Benzeneacetamide, N-[2-[[2-chloro-4,6-dicyano-3,5-bis(propylamino)phenyl]amino]ethyl]- $\alpha$ -[(3,5-dinitrobenzoyl)amino]-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

### RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 27 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:353226 CAPLUS

DN 135:204907

TI Identification of peptides inhibitory to recombinant cysteine proteinase, CPB, of Leishmania mexicana

AU Alves, L. C.; St. Hilaire, P. M.; Meldal, M.; Sanderson, S. J.; Mottram, J. C.; Coombs, G. H.; Juliano, L.; Juliano, M. A.

CS Escola Paulista de Medicina, Department of Biophysics, Universidade Federal de Sao Paulo, Sao Paulo, 04044-20, Brazil

SO Molecular and Biochemical Parasitology (2001), 114(1), 81-88 CODEN: MBIPDP; ISSN: 0166-6851

PB Elsevier Science Ireland Ltd.

DT Journal

LA English

The authors have identified peptides that are relatively resistant to AB hydrolysis by a recombinant cysteine proteinase, CPB2.8ACTE, of Leishmania mexicana, and yet exhibit inhibition constant (Ki) values in the nanomolar range. Common to these peptides is a basic-hydrophobichydrophobic motif in the P3-P1 sites, which is also present in the pro-region of the enzyme. A nine-amino acid stretch, FAARYLNGA, which has good homol. to the pro-region of mammalian cathepsin L was identified as the part of the pro-region most likely to interact with the active site of the parasite enzyme. This peptide is not hydrolyzed by CPB2.8ACTE and inhibited it with a Ki of 4  $\mu$ M. Extension of this sequence at both the N- and C-termini and the introduction of ortho-aminobenzoic acid at the N-terminal site reduced the Ki value to 30 nM. The best substrate for CPB2.8ACTE was also well hydrolyzed by cathepsin L; however, the best inhibitor of the parasite enzyme inhibit poorly cathepsin L, with Ki value two order of magnitude higher than against the parasite enzyme. These promising data provide insights into the peculiar specificity of the parasite enzyme and will aid the design of antiparasitic drugs directed against the leishmanial enzyme.

### IT 357959-84-3

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)

(identification of peptides inhibitory to recombinant cysteine proteinase CPB of Leishmania mexicana in relation to design of antiparasitic drugs)

RN 357959-84-3 CAPLUS

CN L-Glutamamide, N-(2-aminobenzoyl)-L-tyrosyl-L-arginyl-L-phenylalanyl-L-phenylalanyl-L-arginyl-L-arginyl-L-arginyl-L-phenylalanyl-N1-[2-[(2,4-

dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

### IT 357959-86-5

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(identification of peptides inhibitory to recombinant cysteine proteinase CPB of Leishmania mexicana in relation to design of antiparasitic drugs)

RN 357959-86-5 CAPLUS

CN L-Glutamamide, N2-(2-aminobenzoyl)-L-lysyl-L-leucyl-L-phenylalanyl-L-asparaginyl-L-prolyl-L-lysyl-L-phenylalanyl-N1-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-B

## RE.CNT 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 28 OF 83 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 2001:348958 CAPLUS
- DN 135:163967
- TI Selective Neurotensin-Derived Internally Quenched Fluorogenic Substrates for Neurolysin (EC 3.4.24.16): Comparison with Thimet Oligopeptidase (EC 3.4.24.15) and Neprilysin (EC 3.4.24.11)
- AU Oliveira, Vitor; Campos, Marcelo; Hemerly, Jefferson P.; Ferro, Emer S.; Camargo, Antonio C. M.; Juliano, Maria A.; Juliano, Luiz
- CS Department of Biophysics, Escola Paulista de Medicina, Universidade Federal de Sao Paulo, Sao Paulo, SP, 04044-020, Brazil
- SO Analytical Biochemistry (2001), 292(2), 257-265 CODEN: ANBCA2; ISSN: 0003-2697
- PB Academic Press
- DT Journal
- LA English
- AB Internally quenched fluorescent peptides derived from neurotensin (pELYENKPRRPYIL) sequence were synthesized and assayed as substrates for neurolysin (EC 3.4.24.16), thimet oligopeptidase (EC 3.4.24.15 or TOP), and neprilysin (EC 3.4.24.11 or NEP). Abz-LYENKPRRPYILQ-EDDnp (where EDDnp is N-(2,4-dinitrophenyl)ethylenediamine and Abz is ortho-aminobenzoic acid) was derived from neurotensin by the introduction of Q-EDDnp at the C-terminal end of peptide and by the substitution of the pyroglutamic (pE) residue at N-terminus for Abz and a series of shorter